

$P1$

C_1^1

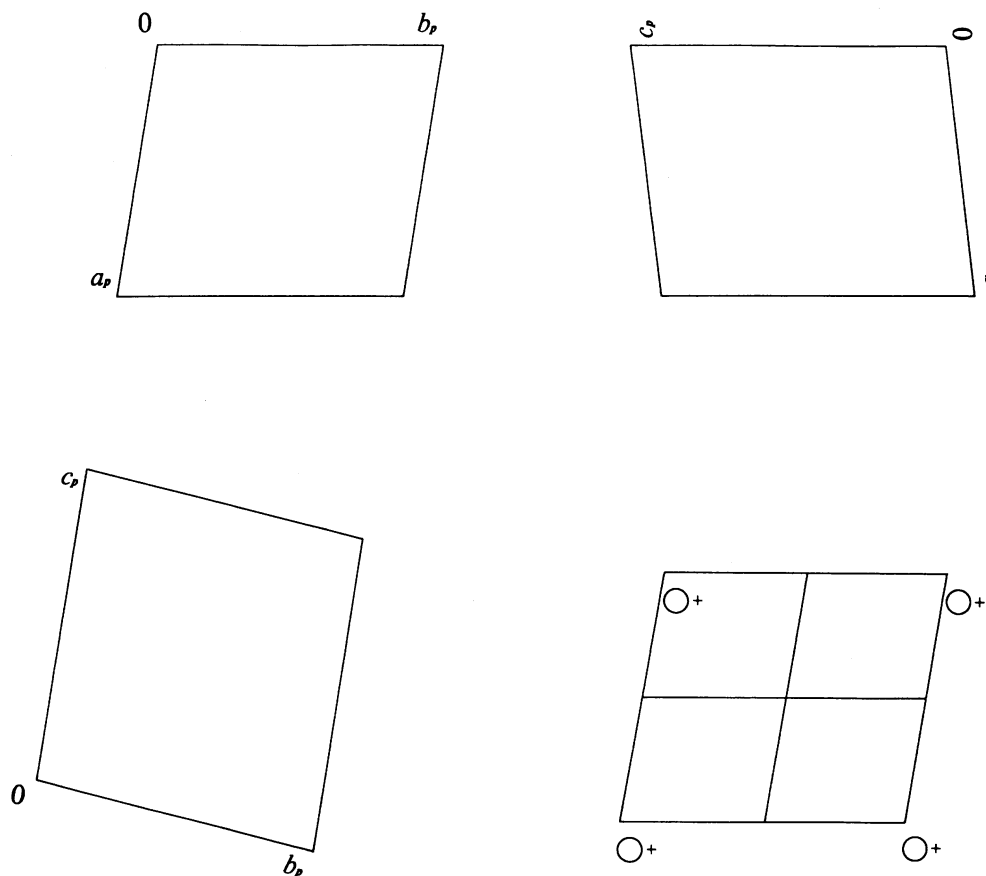
1

Triclinic

No. 1

$P1$

Patterson symmetry $P\bar{1}$



Drawings for type II cell. Proper cell reduction (Chapter 9.2) gives either a type I (α, β, γ acute) or a type II (α, β, γ non-acute) cell.

Origin arbitrary

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

(1) 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
1 a 1	(1) x,y,z	General: no conditions

Symmetry of special projections

Along [001] $p1$ $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$ Origin at 0,0, z	Along [100] $p1$ $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}_p$ Origin at $x,0,0$	Along [010] $p1$ $\mathbf{a}' = \mathbf{c}_p$ $\mathbf{b}' = \mathbf{a}_p$ Origin at 0, $y,0$
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Maximal non-isomorphic subgroups

- I** none
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

- IIc** [2] $P1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{b}' = \mathbf{b} + \mathbf{c}$, $\mathbf{c}' = -\mathbf{b} + \mathbf{c}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{c}$, $\mathbf{c}' = \mathbf{a} + \mathbf{c}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{b} + \mathbf{c}$, $\mathbf{b}' = \mathbf{a} + \mathbf{c}$, $\mathbf{c}' = \mathbf{a} + \mathbf{b}$) (1)

Minimal non-isomorphic supergroups

- I** [2] $P\bar{1}$ (2); [2] $P2$ (3); [2] $P2_1$ (4); [2] $C2$ (5); [2] Pm (6); [2] Pc (7); [2] Cm (8); [2] Cc (9); [3] $P3$ (143); [3] $P3_1$ (144); [3] $P3_2$ (145); [3] $R3$ (146)
II none

$P\bar{1}$

C_i^1

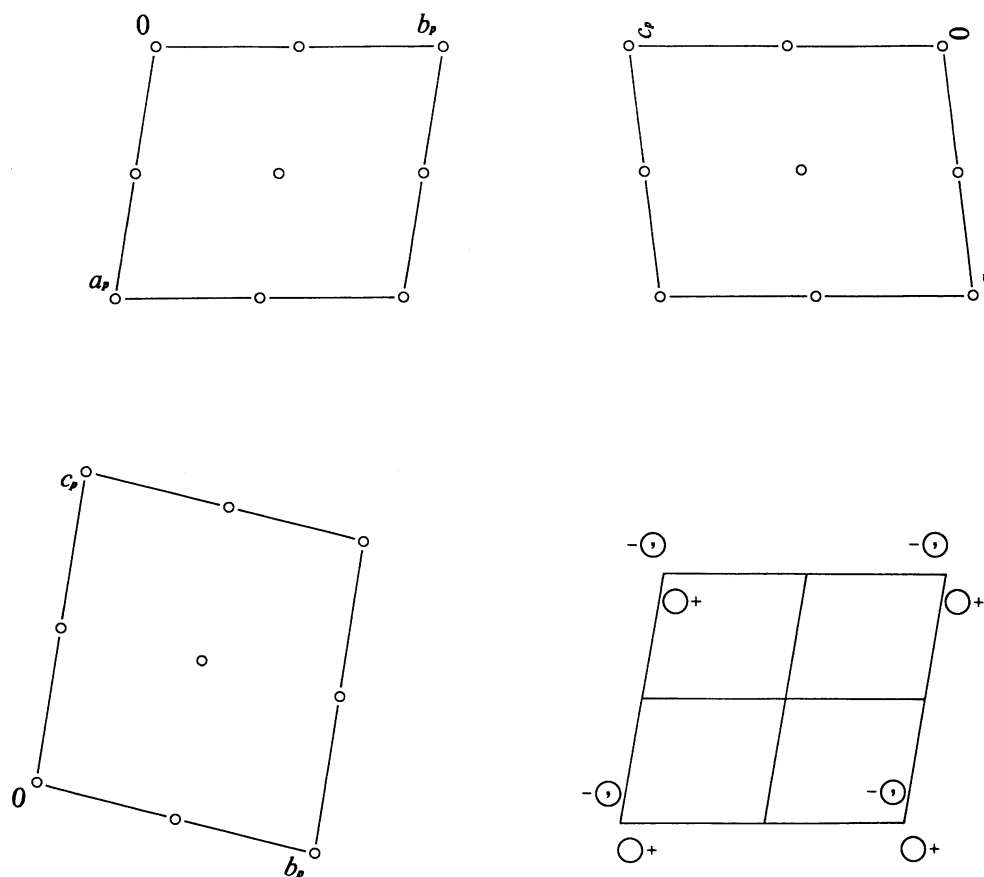
$\bar{1}$

Triclinic

No. 2

$P\bar{1}$

Patterson symmetry $P\bar{1}$



Drawings for type II cell. Proper cell reduction (Chapter 9.2) gives either a type I (α, β, γ acute) or a type II (α, β, γ non-acute) cell.

Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $\bar{1}$ 0,0,0

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions	
2	i	1	(1) x, y, z (2) $\bar{x}, \bar{y}, \bar{z}$	General: no conditions Special: no extra conditions
1	h	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
1	g	$\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	
1	f	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	
1	e	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	
1	d	$\bar{1}$	$\frac{1}{2}, 0, 0$	
1	c	$\bar{1}$	$0, \frac{1}{2}, 0$	
1	b	$\bar{1}$	$0, 0, \frac{1}{2}$	
1	a	$\bar{1}$	$0, 0, 0$	

Symmetry of special projections

Along $[001]$ $p2$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$
 Origin at $0, 0, z$

Along $[100]$ $p2$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x, 0, 0$

Along $[010]$ $p2$
 $\mathbf{a}' = \mathbf{c}_p$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I $[2] P1 (1)$ 1

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2] P\bar{1}$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{b}' = \mathbf{b} + \mathbf{c}, \mathbf{c}' = -\mathbf{b} + \mathbf{c}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b}$) (2)

Minimal non-isomorphic supergroups

I $[2] P2/m (10)$; $[2] P2_1/m (11)$; $[2] C2/m (12)$; $[2] P2/c (13)$; $[2] P2_1/c (14)$; $[2] C2/c (15)$; $[3] P\bar{3} (147)$; $[3] R\bar{3} (148)$

II none

$P2$

C_2^1

2

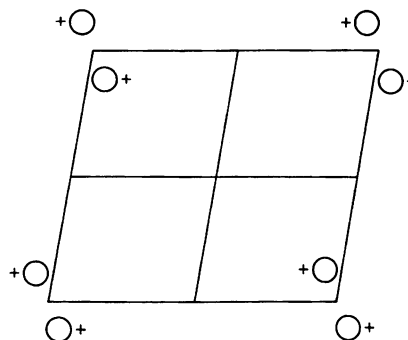
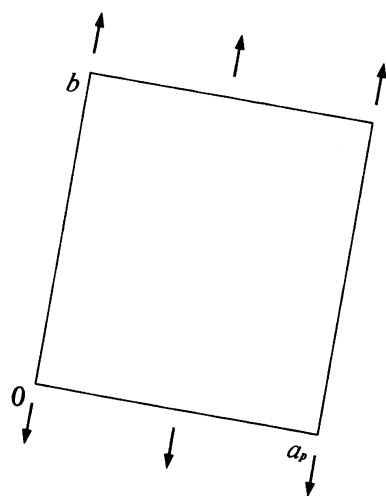
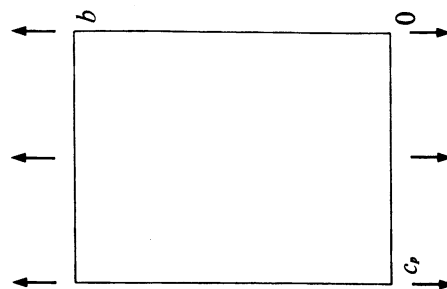
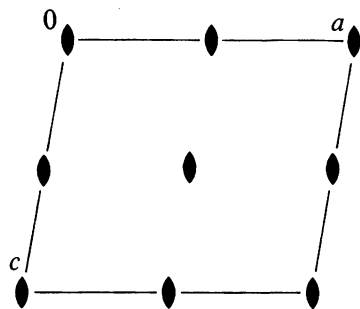
Monoclinic

No. 3

$P121$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin on 2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0, y, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
2 <i>e</i> 1	(1) x,y,z	(2) \bar{x},y,\bar{z}	General: no conditions Special: no extra conditions
1 <i>d</i> 2	$\frac{1}{2},y,\frac{1}{2}$		
1 <i>c</i> 2	$\frac{1}{2},y,0$		
1 <i>b</i> 2	$0,y,\frac{1}{2}$		
1 <i>a</i> 2	$0,y,0$		

Symmetry of special projections

Along [001] $p1m1$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $p11m$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x,0,0$

Along [010] $p2$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1(1)$ 1

IIa none

IIb [2] $P12_11$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_1, 4$); [2] $C121$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($C2, 5$); [2] $A121$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2, 5$);
 [2] $F121$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2, 5$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P121$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2, 3$); [2] $P121$ ($\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$) ($P2, 3$)

Minimal non-isomorphic supergroups

I [2] $P2/m$ (10); [2] $P2/c$ (13); [2] $P222$ (16); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $C222$ (21); [2] $Pmm2$ (25); [2] $Pcc2$ (27);
 [2] $Pma2$ (28); [2] $Pnc2$ (30); [2] $Pba2$ (32); [2] $Pnn2$ (34); [2] $Cmm2$ (35); [2] $Ccc2$ (37); [2] $P4$ (75); [2] $P4_2$ (77);
 [2] $P\bar{4}$ (81); [3] $P6$ (168); [3] $P6_2$ (171); [3] $P6_4$ (172)

II [2] $C121$ ($C2, 5$); [2] $A121$ ($C2, 5$); [2] $I121$ ($C2, 5$)

$P2$

C_2^1

2

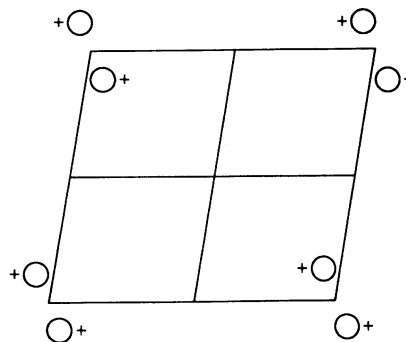
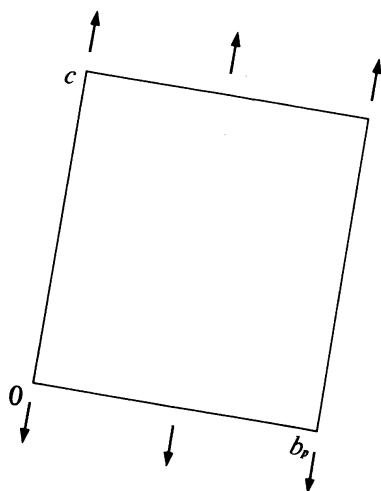
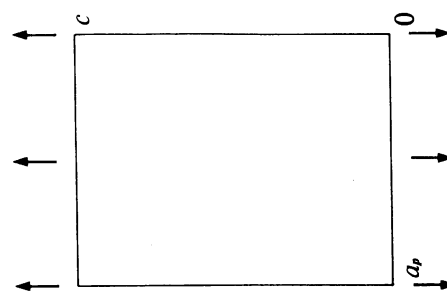
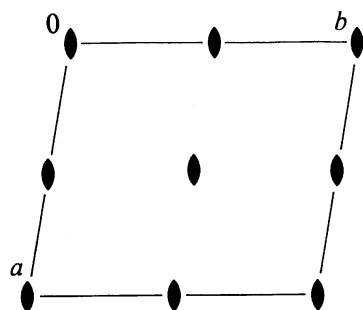
Monoclinic

No. 3

$P112$

Patterson symmetry $P112/m$

UNIQUE AXIS c



Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
2 <i>e</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	General: no conditions Special: no extra conditions
1 <i>d</i> 2	$\frac{1}{2}, \frac{1}{2}, z$		
1 <i>c</i> 2	$0, \frac{1}{2}, z$		
1 <i>b</i> 2	$\frac{1}{2}, 0, z$		
1 <i>a</i> 2	$0, 0, z$		

Symmetry of special projections

Along [001] $p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P1(1)$ 1

IIa none

IIb [2] $P112_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1, 4$); [2] $A112$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2, 5$); [2] $B112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C2, 5$);
 [2] $F112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2, 5$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P112$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2, 3$); [2] $P112$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) ($P2, 3$)

Minimal non-isomorphic supergroups

I [2] $P2/m$ (10); [2] $P2/c$ (13); [2] $P222$ (16); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $C222$ (21); [2] $Pmm2$ (25); [2] $Pcc2$ (27);
 [2] $Pma2$ (28); [2] $Pnc2$ (30); [2] $Pba2$ (32); [2] $Pnn2$ (34); [2] $Cmm2$ (35); [2] $Ccc2$ (37); [2] $P4$ (75); [2] $P4_2$ (77);
 [2] $P\bar{4}$ (81); [3] $P6$ (168); [3] $P6_2$ (171); [3] $P6_4$ (172)

II [2] $A112$ ($C2, 5$); [2] $B112$ ($C2, 5$); [2] $I112$ ($C2, 5$)

$P2_1$

C_2^2

2

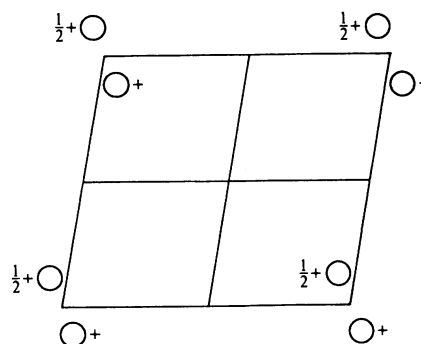
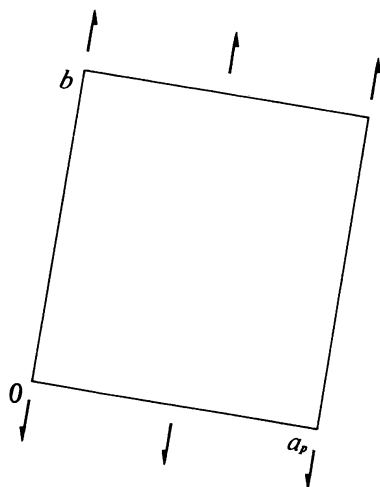
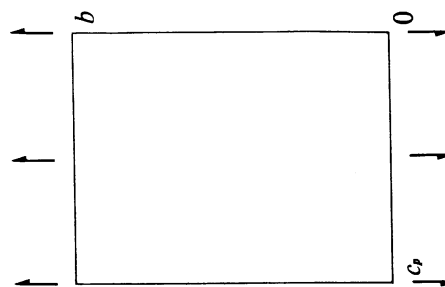
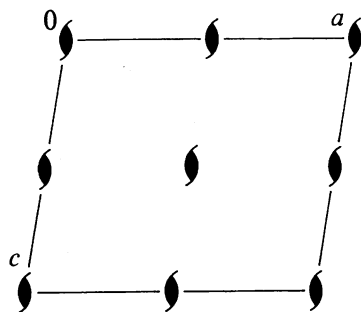
Monoclinic

No. 4

$P12_11$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin on 2_1

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1 (2) $2(0, \frac{1}{2}, 0) 0, y, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x, y, z (2) $\bar{x}, y + \frac{1}{2}, \bar{z}$	$0k0 : k = 2n$

Symmetry of special projections

Along [001] $p1g1$	Along [100] $p11g$	Along [010] $p2$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$	$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0, 0, z$	Origin at $x, 0, 0$	Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P1(1)$ 1

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIIc [2] $P12_11$ ($\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$) ($P2_1, 4$); [3] $P12_11$ ($\mathbf{b}' = 3\mathbf{b}$) ($P2_1, 4$)

Minimal non-isomorphic supergroups

I [2] $P2_1/m$ (11); [2] $P2_1/c$ (14); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $P2_12_12_1$ (19); [2] $C222_1$ (20); [2] $Pmc2_1$ (26); [2] $Pca2_1$ (29); [2] $Pmn2_1$ (31); [2] $Pna2_1$ (33); [2] $Cmc2_1$ (36); [2] $P4_1$ (76); [2] $P4_3$ (78); [3] $P6_1$ (169); [3] $P6_5$ (170); [3] $P6_3$ (173)

II [2] $C121$ ($C2, 5$); [2] $A121$ ($C2, 5$); [2] $I121$ ($C2, 5$); [2] $P121$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P2, 3$)

$P2_1$

No. 4

C_2^2

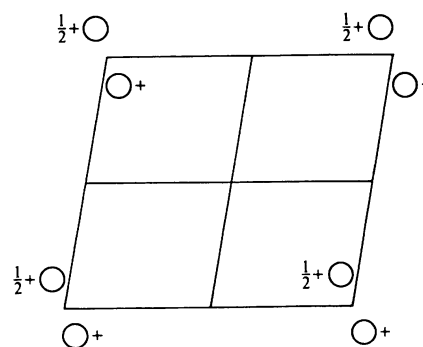
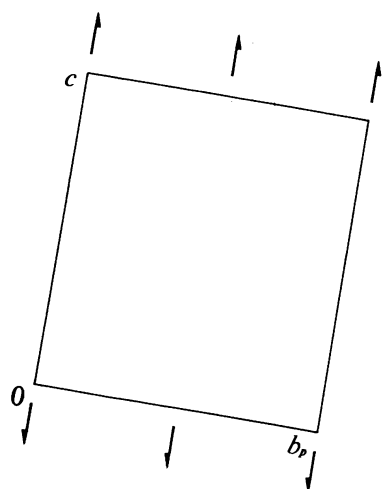
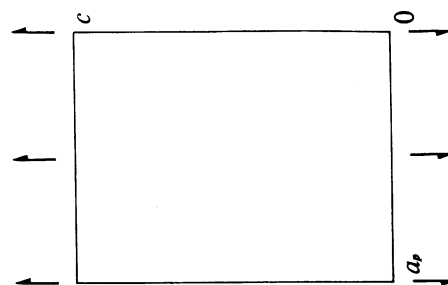
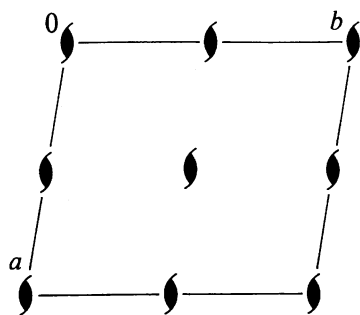
$P112_1$

2

Monoclinic

Patterson symmetry $P112/m$

UNIQUE AXIS c



Origin on 2_1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2}) 0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x, y, z (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	$00l : l = 2n$

Symmetry of special projections

Along [001] $p2$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$	Along [100] $p1g1$ $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [010] $p1g$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$ Origin at $0, y, 0$
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Maximal non-isomorphic subgroups

I [2] $P1(1)$ 1

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P112_1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) ($P2_1, 4$); [3] $P112_1$ ($\mathbf{c}' = 3\mathbf{c}$) ($P2_1, 4$)

Minimal non-isomorphic supergroups

I [2] $P2_1/m$ (11); [2] $P2_1/c$ (14); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $P2_12_12_1$ (19); [2] $C222_1$ (20); [2] $Pmc2_1$ (26); [2] $Pca2_1$ (29); [2] $Pmn2_1$ (31); [2] $Pna2_1$ (33); [2] $Cmc2_1$ (36); [2] $P4_1$ (76); [2] $P4_3$ (78); [3] $P6_1$ (169); [3] $P6_5$ (170); [3] $P6_3$ (173)

II [2] $A112$ ($C2, 5$); [2] $B112$ ($C2, 5$); [2] $I112$ ($C2, 5$); [2] $P112$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2, 3$)

$C2$

C_2^3

2

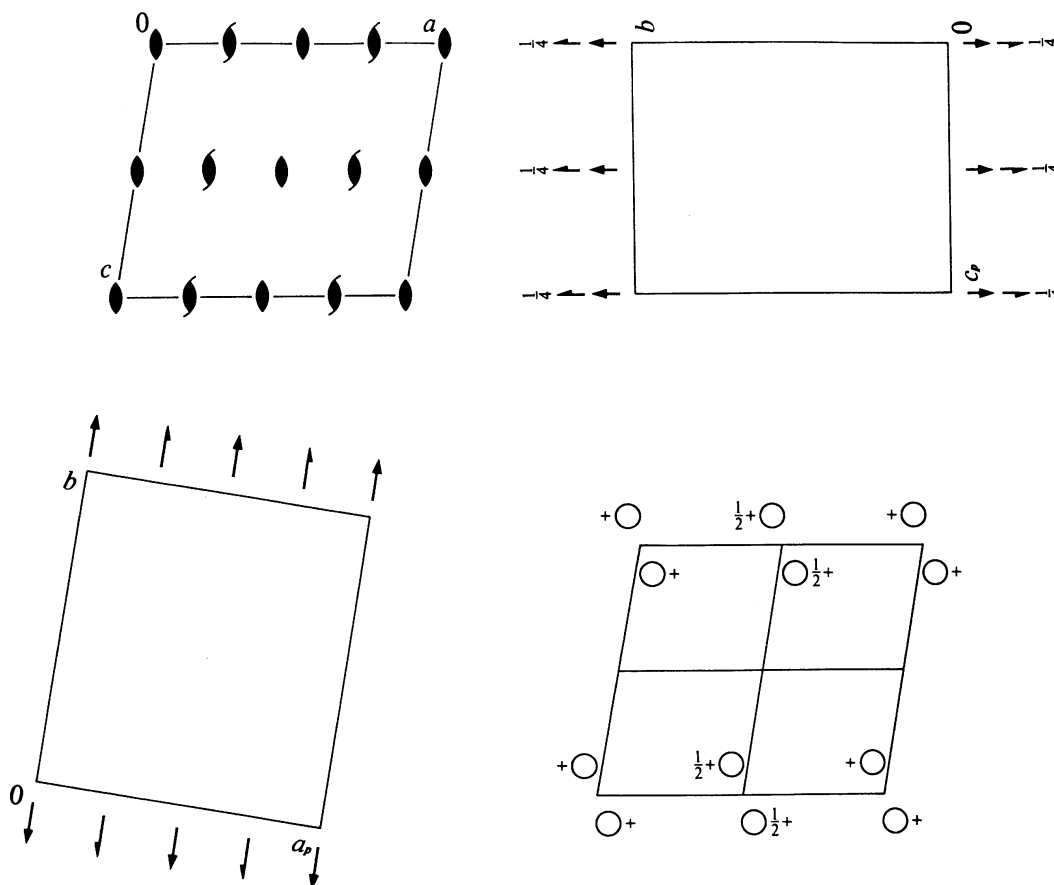
Monoclinic

No. 5

$C121$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2 \ 0,y,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,\frac{1}{2},0) \ \frac{1}{4},y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$	General:
4	<i>c</i> 1	(1) x,y,z (2) \bar{x},y,\bar{z}	$hkl : h+k=2n$ $h0l : h=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$
			Special: no extra conditions
2	<i>b</i> 2	$0,y,\frac{1}{2}$	
2	<i>a</i> 2	$0,y,0$	

Symmetry of special projections

Along $[001]$ $c1m1$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along $[100]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along $[010]$ $p2$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

- I** [2] $C1(P1, 1)$ 1+
- IIa** [2] $P12_11(P2_1, 4)$ 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$
[2] $P121(P2, 3)$ 1; 2
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [2] $C121(\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = \mathbf{a} + 2\mathbf{c}, \mathbf{c}' = 2\mathbf{c})(C2, 5)$; [3] $C121(\mathbf{b}' = 3\mathbf{b})(C2, 5)$

Minimal non-isomorphic supergroups

- I** [2] $C2/m(12)$; [2] $C2/c(15)$; [2] $C222_1(20)$; [2] $C222(21)$; [2] $F222(22)$; [2] $I222(23)$; [2] $I2_12_12_1(24)$; [2] $Amm2(38)$;
[2] $Aem2(39)$; [2] $Ama2(40)$; [2] $Aea2(41)$; [2] $Fmm2(42)$; [2] $Fdd2(43)$; [2] $Imm2(44)$; [2] $Iba2(45)$; [2] $Ima2(46)$;
[2] $I4(79)$; [2] $I4_1(80)$; [2] $I\bar{4}(82)$; [3] $P312(149)$; [3] $P321(150)$; [3] $P3_112(151)$; [3] $P3_121(152)$; [3] $P3_212(153)$;
[3] $P3_221(154)$; [3] $R32(155)$
- II** [2] $P121(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b})(P2, 3)$

C_2

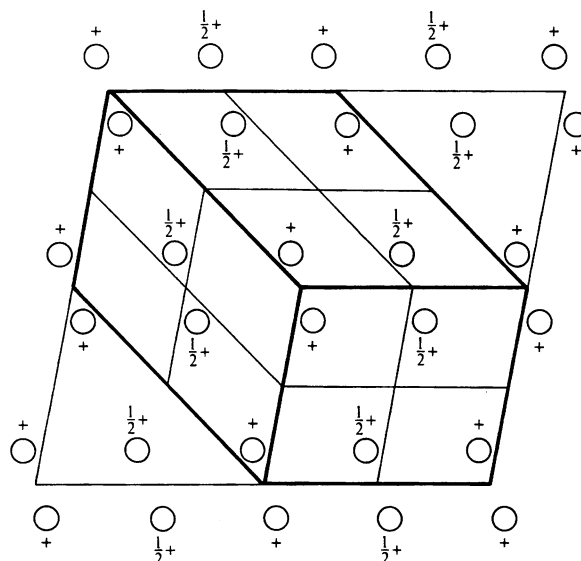
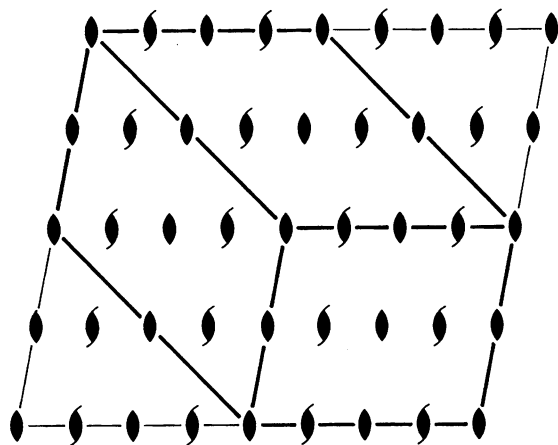
C_2^3

2

Monoclinic

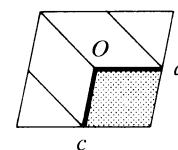
No. 5

UNIQUE AXIS b , DIFFERENT CELL CHOICES



C_{121}

UNIQUE AXIS b , CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Generators selected $(1); t(1,0,0); t(0,1,0); t(0,0,1); t(\frac{1}{2}, \frac{1}{2}, 0); (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, 0) +$

4	c	1	(1) x, y, z	(2) \bar{x}, y, \bar{z}
---	-----	---	---------------	---------------------------

Reflection conditions

General:

$hkl : h + k = 2n$
 $h0l : h = 2n$
 $0kl : k = 2n$
 $hk0 : h + k = 2n$
 $0k0 : k = 2n$
 $h00 : h = 2n$

Special: no extra conditions

2	b	2	$0, y, \frac{1}{2}$
---	-----	---	---------------------

2	a	2	$0, y, 0$
---	-----	---	-----------

A121

UNIQUE AXIS b , CELL CHOICE 2

Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

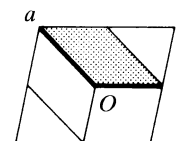
Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

4	c	1	(1) x,y,z	(2) \bar{x},y,\bar{z}
---	-----	---	-------------	-------------------------

2	b	2	$\frac{1}{2}, y, \frac{1}{2}$
---	-----	---	-------------------------------

2	a	2	$0, y, 0$
---	-----	---	-----------



Reflection conditions

General:

$$hkl : k + l = 2n$$

$$h0l : l = 2n$$

$$0kl : k + l = 2n$$

$$hk0 : k = 2n$$

$$0k0 : k = 2n$$

$$00l : l = 2n$$

Special: no extra conditions

I121

UNIQUE AXIS b , CELL CHOICE 3

Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2)

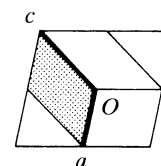
Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

4	c	1	(1) x,y,z	(2) \bar{x},y,\bar{z}
---	-----	---	-------------	-------------------------

2	b	2	$\frac{1}{2}, y, 0$
---	-----	---	---------------------

2	a	2	$0, y, 0$
---	-----	---	-----------



Reflection conditions

General:

$$hkl : h + k + l = 2n$$

$$h0l : h + l = 2n$$

$$0kl : k + l = 2n$$

$$hk0 : h + k = 2n$$

$$0k0 : k = 2n$$

$$h00 : h = 2n$$

$$00l : l = 2n$$

Special: no extra conditions

C_2

C_2^3

2

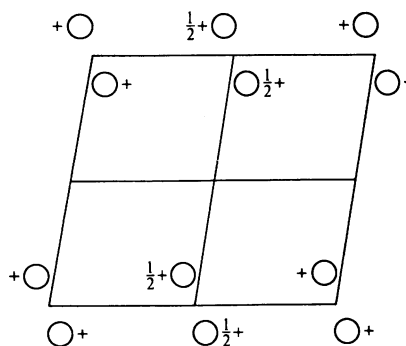
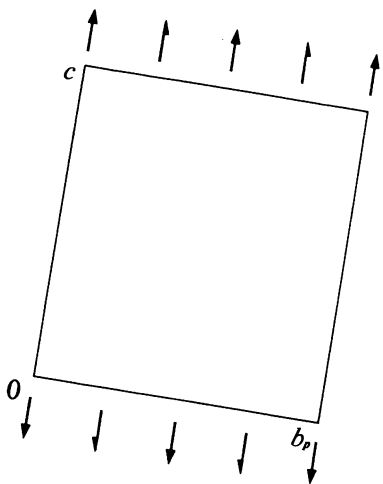
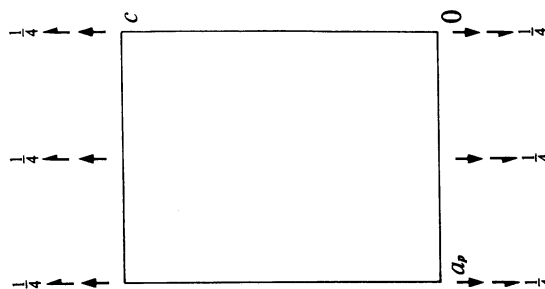
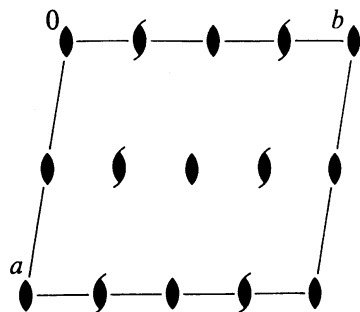
Monoclinic

No. 5

A112

Patterson symmetry A112/m

UNIQUE AXIS c , CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1
- (2) $2 \ 0,0,z$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) $t(0, \frac{1}{2}, \frac{1}{2})$
- (2) $2(0,0, \frac{1}{2}) \ 0, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	General:
4	<i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	$hkl : k+l=2n$ $hk0 : k=2n$ $0kl : k+l=2n$ $h0l : l=2n$ $00l : l=2n$ $0k0 : k=2n$
				Special: no extra conditions
2	<i>b</i> 2	$\frac{1}{2},0,z$		
2	<i>a</i> 2	$0,0,z$		

Symmetry of special projections

Along $[001]$ $p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0,0,z$

Along $[100]$ $c1m1$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along $[010]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at $0,y,0$

Maximal non-isomorphic subgroups

- I** [2] $A1 (P1, 1)$ 1+
- IIa** [2] $P112_1 (P2_1, 4)$ 1; $2 + (0, \frac{1}{2}, \frac{1}{2})$
 [2] $P112 (P2, 3)$ 1; 2
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [2] $A112 (\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}) (C2, 5)$; [3] $A112 (\mathbf{c}' = 3\mathbf{c}) (C2, 5)$

Minimal non-isomorphic supergroups

- I** [2] $C2/m (12)$; [2] $C2/c (15)$; [2] $C222_1 (20)$; [2] $C222 (21)$; [2] $F222 (22)$; [2] $I222 (23)$; [2] $I2_12_12_1 (24)$; [2] $Amm2 (38)$;
 [2] $Aem2 (39)$; [2] $Ama2 (40)$; [2] $Aea2 (41)$; [2] $Fmm2 (42)$; [2] $Fdd2 (43)$; [2] $Imm2 (44)$; [2] $Iba2 (45)$; [2] $Ima2 (46)$;
 [2] $I4 (79)$; [2] $I4_1 (80)$; [2] $I\bar{4} (82)$; [3] $P312 (149)$; [3] $P321 (150)$; [3] $P3_112 (151)$; [3] $P3_21 (152)$; [3] $P3_212 (153)$;
 [3] $P3_221 (154)$; [3] $R32 (155)$
- II** [2] $P112 (\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2, 3)$

C_2

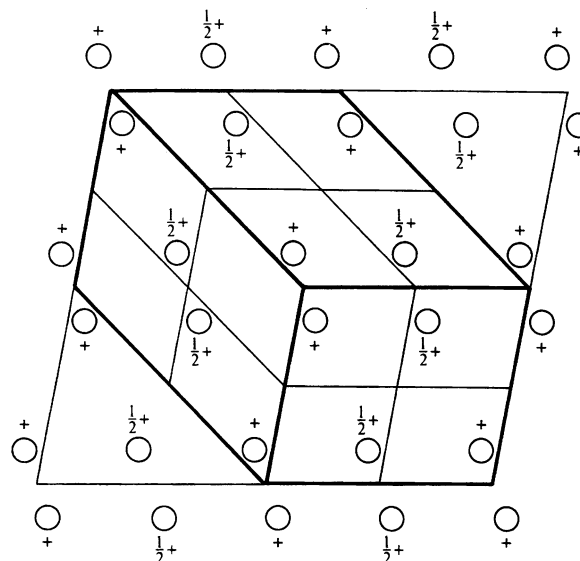
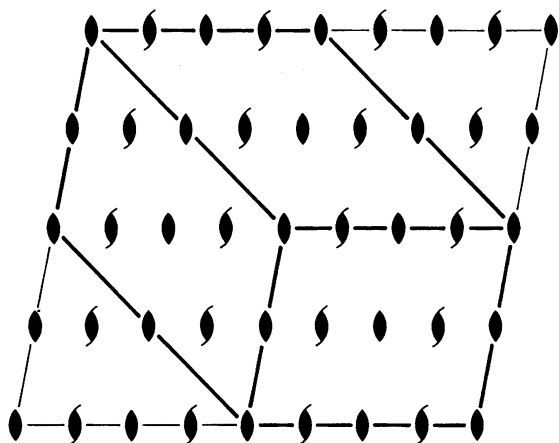
C_2^3

2

Monoclinic

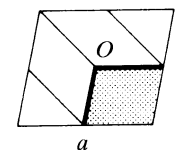
No. 5

UNIQUE AXIS c , DIFFERENT CELL CHOICES



A112

UNIQUE AXIS c , CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (0, \frac{1}{2}, \frac{1}{2}) +$

4	c	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z
---	-----	---	---------------	---------------------------

Reflection conditions

General:

$hkl : k + l = 2n$
 $hk0 : k = 2n$
 $0kl : k + l = 2n$
 $h0l : l = 2n$
 $00l : l = 2n$
 $0k0 : k = 2n$

Special: no extra conditions

2	b	2	$\frac{1}{2}, 0, z$
---	-----	---	---------------------

2	a	2	$0, 0, z$
---	-----	---	-----------

B112UNIQUE AXIS c , CELL CHOICE 2**Origin** on 2**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},0,\frac{1}{2}) +$

4	c	1	(1) x,y,z	(2) \bar{x},\bar{y},z
---	-----	---	-------------	-------------------------

2	b	2	$\frac{1}{2},\frac{1}{2},z$
---	-----	---	-----------------------------

2	a	2	$0,0,z$
---	-----	---	---------

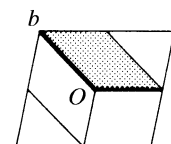
I112UNIQUE AXIS c , CELL CHOICE 3**Origin** on 2**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$

4	c	1	(1) x,y,z	(2) \bar{x},\bar{y},z
---	-----	---	-------------	-------------------------

2	b	2	$0,\frac{1}{2},z$
---	-----	---	-------------------

2	a	2	$0,0,z$
---	-----	---	---------



Reflection conditions

General:

$hkl : h + l = 2n$

$hk0 : h = 2n$

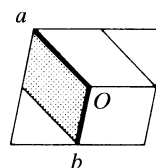
$0kl : l = 2n$

$h0l : h + l = 2n$

$00l : l = 2n$

$h00 : h = 2n$

Special: no extra conditions



Reflection conditions

General:

$hkl : h + k + l = 2n$

$hk0 : h + k = 2n$

$0kl : k + l = 2n$

$h0l : h + l = 2n$

$00l : l = 2n$

$h00 : h = 2n$

$0k0 : k = 2n$

Special: no extra conditions

Pm

C_s^1

m

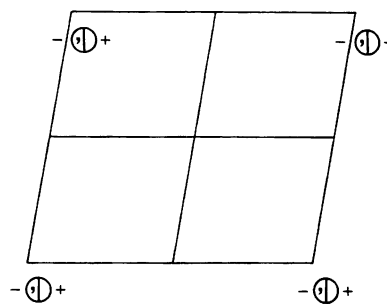
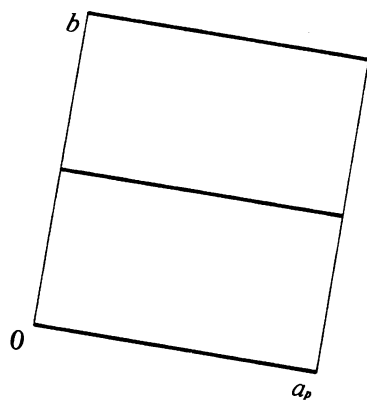
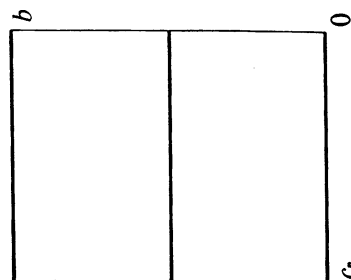
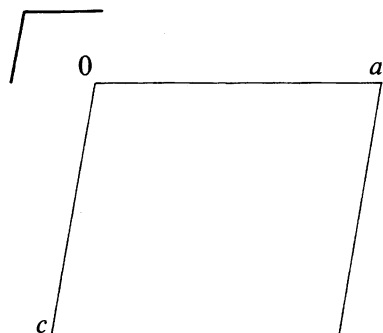
Monoclinic

No. 6

$P1m1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin on mirror plane m

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $m \ x, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
2 <i>c</i> 1	(1) x,y,z	(2) x,\bar{y},z	General: no conditions Special: no extra conditions
1 <i>b</i> <i>m</i>	$x, \frac{1}{2}, z$		
1 <i>a</i> <i>m</i>	$x, 0, z$		

Symmetry of special projections

Along [001] <i>p</i> 1 1 <i>m</i> $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, <i>z</i>	Along [100] <i>p</i> 1 <i>m</i> 1 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$ Origin at <i>x</i> , 0, 0	Along [010] <i>p</i> 1 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0, <i>y</i> , 0
--	---	--

Maximal non-isomorphic subgroups

I [2] *P* 1 (1) 1

IIa none

IIb [2] *P* 1 *c* 1 ($\mathbf{c}' = 2\mathbf{c}$) (*Pc*, 7); [2] *P* 1 *a* 1 ($\mathbf{a}' = 2\mathbf{a}$) (*Pc*, 7); [2] *B* 1 *e* 1 ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) (*Pc*, 7); [2] *C* 1 *m* 1 ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (*Cm*, 8); [2] *A* 1 *m* 1 ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (*Cm*, 8); [2] *F* 1 *m* 1 ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (*Cm*, 8)

Maximal isomorphic subgroups of lowest index

IIc [2] *P* 1 *m* 1 ($\mathbf{b}' = 2\mathbf{b}$) (*Pm*, 6); [2] *P* 1 *m* 1 ($\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$) (*Pm*, 6)

Minimal non-isomorphic supergroups

I [2] *P* 2/*m* (10); [2] *P* 2₁/*m* (11); [2] *P* *m* *m* 2 (25); [2] *P* *m* *c* 2₁ (26); [2] *P* *m* *a* 2 (28); [2] *P* *m* *n* 2₁ (31); [2] *A* *m* *m* 2 (38); [2] *A* *m* *a* 2 (40); [3] *P* $\bar{6}$ (174)

II [2] *C* 1 *m* 1 (*Cm*, 8); [2] *A* 1 *m* 1 (*Cm*, 8); [2] *I* 1 *m* 1 (*Cm*, 8)

Pm

No. 6

C_s^1

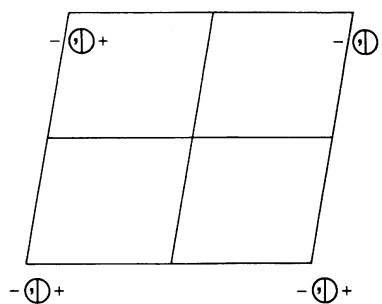
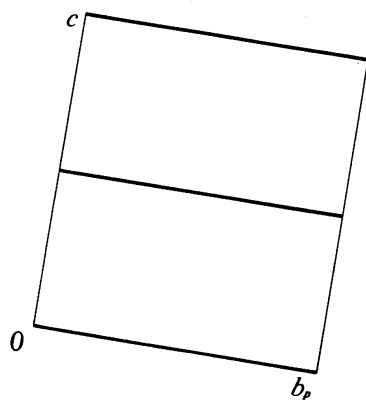
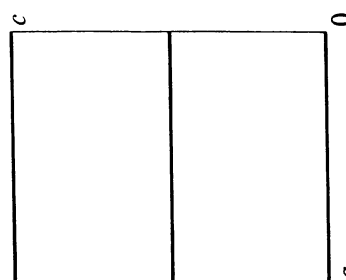
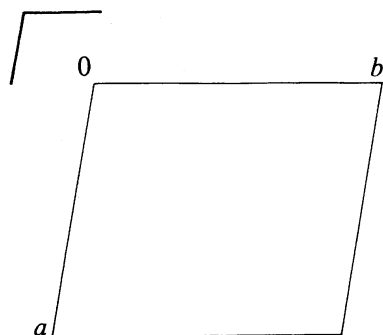
$P11m$

m

Monoclinic

Patterson symmetry $P112/m$

UNIQUE AXIS c



Origin on mirror plane m

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1 (2) $m \ x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
2 <i>c</i> 1	(1) x,y,z	(2) x,y,\bar{z}	General: no conditions Special: no extra conditions
1 <i>b</i> <i>m</i>	$x,y,\frac{1}{2}$		
1 <i>a</i> <i>m</i>	$x,y,0$		

Symmetry of special projections

Along [001] <i>p</i> 1 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [100] <i>p</i> 1 1 <i>m</i> $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [010] <i>p</i> 1 <i>m</i> 1 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$ Origin at 0, $y, 0$
--	---	---

Maximal non-isomorphic subgroups

I [2] *P* 1 (1) 1

IIa none

IIb [2] *P* 1 1 *a* ($\mathbf{a}' = 2\mathbf{a}$) (*Pc*, 7); [2] *P* 1 1 *b* ($\mathbf{b}' = 2\mathbf{b}$) (*Pc*, 7); [2] *C* 1 1 *e* ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (*Pc*, 7); [2] *A* 1 1 *m* ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (*Cm*, 8); [2] *B* 1 1 *m* ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) (*Cm*, 8); [2] *F* 1 1 *m* ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (*Cm*, 8)

Maximal isomorphic subgroups of lowest index

IIc [2] *P* 1 1 *m* ($\mathbf{c}' = 2\mathbf{c}$) (*Pm*, 6); [2] *P* 1 1 *m* ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) (*Pm*, 6)

Minimal non-isomorphic supergroups

I [2] *P* 2/*m* (10); [2] *P* 2₁/*m* (11); [2] *Pmm* 2 (25); [2] *Pmc* 2₁ (26); [2] *Pma* 2 (28); [2] *Pmn* 2₁ (31); [2] *Amm* 2 (38); [2] *Ama* 2 (40); [3] *P* $\bar{6}$ (174)

II [2] *A* 1 1 *m* (*Cm*, 8); [2] *B* 1 1 *m* (*Cm*, 8); [2] *I* 1 1 *m* (*Cm*, 8)

Pc

C_s^2

m

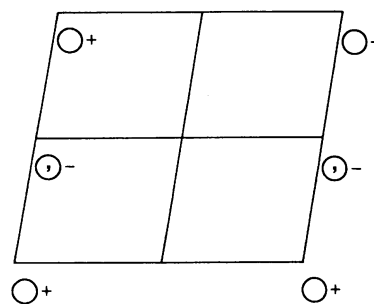
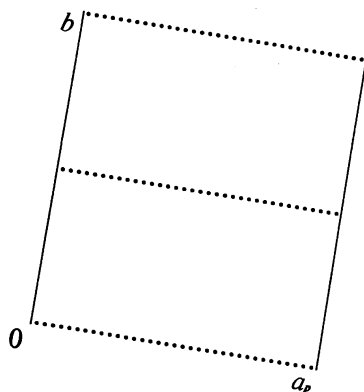
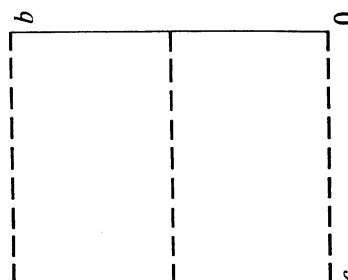
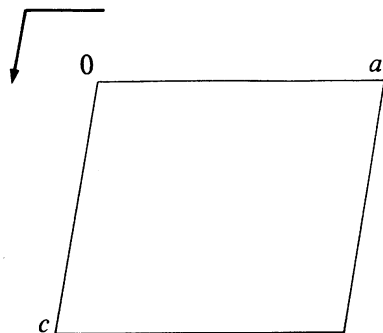
Monoclinic

No. 7

$P1c1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $c \ x, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 <i>a</i> 1	(1) x, y, z (2) $x, \bar{y}, z + \frac{1}{2}$	$h0l : l = 2n$ $00l : l = 2n$

Symmetry of special projections

Along [001] $p11m$ $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [100] $p1g1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$ Origin at $x, 0, 0$	Along [010] $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0, $y, 0$
--	--	---

Maximal non-isomorphic subgroups

- I** [2] $P1(1)$ 1
IIa none
IIb [2] $C1c1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($Cc, 9$)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $P1c1$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pc, 7$); [2] $P1c1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$) ($Pc, 7$)

Minimal non-isomorphic supergroups

- I** [2] $P2/c$ (13); [2] $P2_1/c$ (14); [2] $Pmc2_1$ (26); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pca2_1$ (29); [2] $Pnc2$ (30); [2] $Pmn2_1$ (31);
 [2] $Pba2$ (32); [2] $Pna2_1$ (33); [2] $Pnn2$ (34); [2] $Aem2$ (39); [2] $Aea2$ (41)
II [2] $C1c1$ ($Cc, 9$); [2] $A1m1$ ($Cm, 8$); [2] $I1c1$ ($Cc, 9$); [2] $P1m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pm, 6$)

Pc

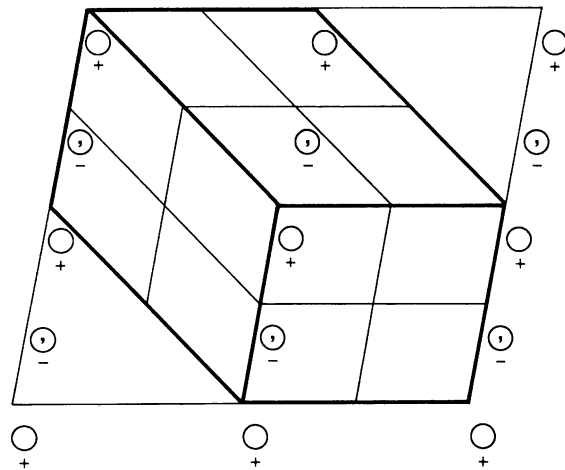
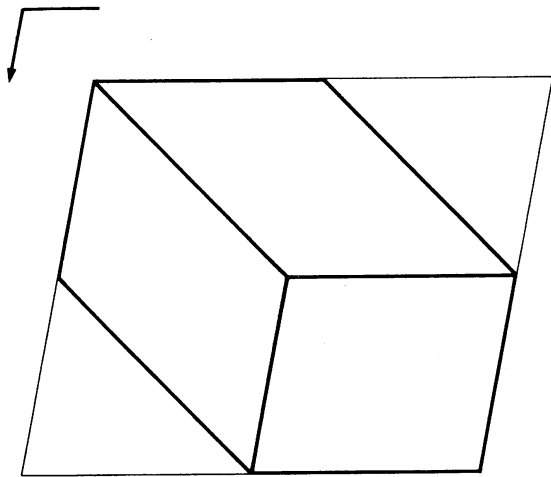
C_s^2

m

Monoclinic

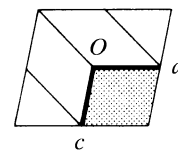
No. 7

UNIQUE AXIS b , DIFFERENT CELL CHOICES



$P1c1$

UNIQUE AXIS b , CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

2 a 1

(1) x, y, z

(2) $x, \bar{y}, z + \frac{1}{2}$

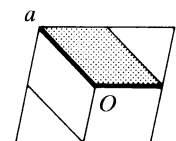
General:

$h0l : l = 2n$

$00l : l = 2n$

P1n1UNIQUE AXIS *b*, CELL CHOICE 2**Origin** on glide plane *n***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

2 *a* 1 (1) x, y, z (2) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ 

Reflection conditions

General:

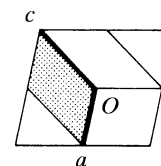
$$h0l : h + l = 2n$$

$$h00 : h = 2n$$

$$00l : l = 2n$$

P1a1UNIQUE AXIS *b*, CELL CHOICE 3**Origin** on glide plane *a***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

2 *a* 1 (1) x, y, z (2) $x + \frac{1}{2}, \bar{y}, z$ 

Reflection conditions

General:

$$h0l : h = 2n$$

$$h00 : h = 2n$$

Pc

C_s^2

m

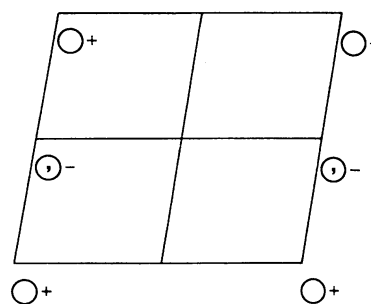
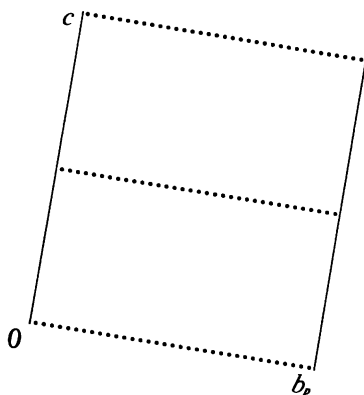
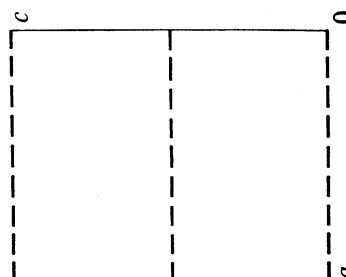
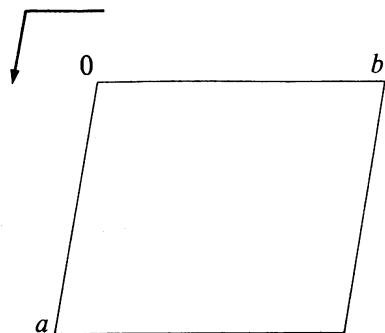
Monoclinic

No. 7

$P11a$

Patterson symmetry $P112/m$

UNIQUE AXIS c , CELL CHOICE 1



Origin on glide plane a

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- (1) 1
- (2) a $x, y, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $x + \frac{1}{2}, y, \bar{z}$	$hk0 : h = 2n$ $h00 : h = 2n$

Symmetry of special projections

Along [001] $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [100] $p11m$ $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [010] $p1g1$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$ Origin at 0, y, 0
---	--	--

Maximal non-isomorphic subgroups

- I** [2] $P1(1)$ 1
IIa none
IIb [2] $A11a(\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (Cc, 9)$

Maximal isomorphic subgroups of lowest index

- IIc** [2] $P11a(\mathbf{c}' = 2\mathbf{c}) (Pc, 7)$; [2] $P11a(\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = 2\mathbf{b}) (Pc, 7)$

Minimal non-isomorphic supergroups

- I** [2] $P2/c(13)$; [2] $P2_1/c(14)$; [2] $Pmc2_1(26)$; [2] $Pcc2(27)$; [2] $Pma2(28)$; [2] $Pca2_1(29)$; [2] $Pnc2(30)$; [2] $Pmn2_1(31)$;
 [2] $Pba2(32)$; [2] $Pna2_1(33)$; [2] $Pnn2(34)$; [2] $Aem2(39)$; [2] $Aea2(41)$
II [2] $A11a(Cc, 9)$; [2] $B11m(Cm, 8)$; [2] $I11a(Cc, 9)$; [2] $P11m(\mathbf{a}' = \frac{1}{2}\mathbf{a}) (Pm, 6)$

Pc

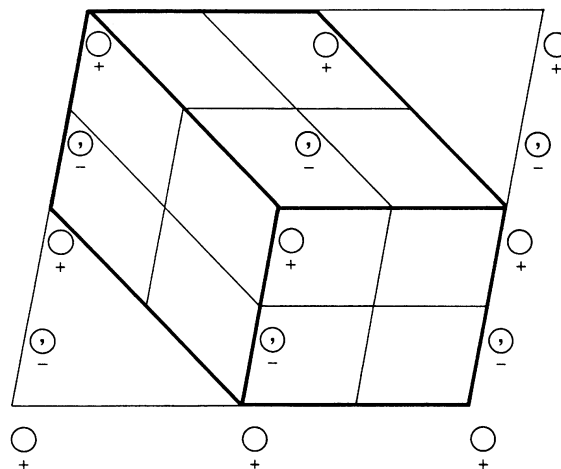
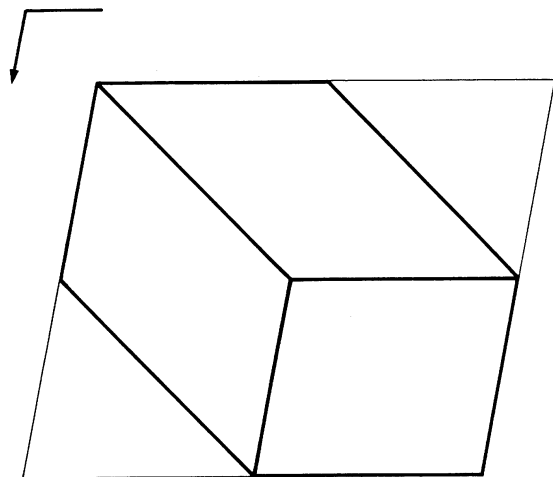
C_s^2

m

Monoclinic

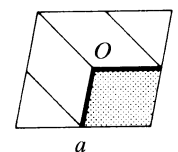
No. 7

UNIQUE AXIS c , DIFFERENT CELL CHOICES



$P11a$

UNIQUE AXIS c , CELL CHOICE 1



Origin on glide plane a

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

2 a 1

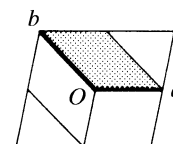
(1) x, y, z

(2) $x + \frac{1}{2}, y, \bar{z}$

General:

$hk0: h = 2n$

$h00: h = 2n$

P11nUNIQUE AXIS *c*, CELL CHOICE 2**Origin** on glide plane *n***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

2 *a* 1 (1) x,y,z (2) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$

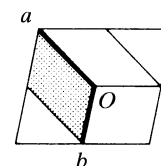
Reflection conditions

General:

$$hk0: h + k = 2n$$

$$h00: h = 2n$$

$$0k0: k = 2n$$

P11bUNIQUE AXIS *c*, CELL CHOICE 3**Origin** on glide plane *b***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

2 *a* 1 (1) x,y,z (2) $x, y + \frac{1}{2}, \bar{z}$

Reflection conditions

General:

$$hk0: k = 2n$$

$$0k0: k = 2n$$

Cm

C_s^3

m

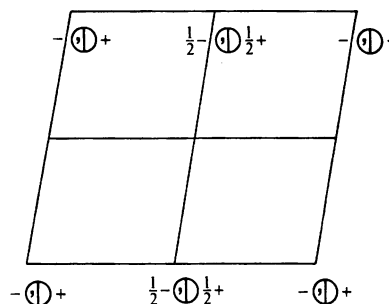
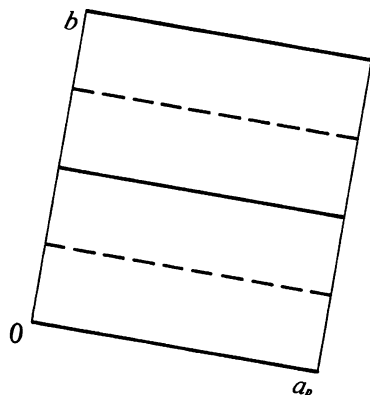
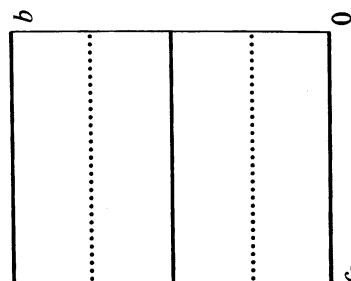
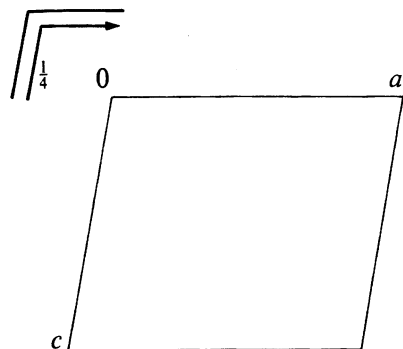
Monoclinic

No. 8

$C1m1$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin on mirror plane m

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $m \ x, 0, z$

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ (2) $a \ x, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
	$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4 <i>b</i> 1	(1) x,y,z	(2) x,\bar{y},z	$hkl : h+k=2n$ $h0l : h=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$
2 <i>a</i> <i>m</i>	$x,0,z$		Special: no extra conditions

Symmetry of special projections

Along [001] $c11m$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x,0,0$

Along [010] $p1$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

- I** [2] $C1(P1, 1)$ 1+
- IIa** [2] $P1a1(Pc, 7)$ 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $P1m1(Pm, 6)$ 1; 2
- IIb** [2] $C1c1(\mathbf{c}' = 2\mathbf{c})(Cc, 9)$; [2] $I1c1(\mathbf{c}' = 2\mathbf{c})(Cc, 9)$

Maximal isomorphic subgroups of lowest index

- IIc** [2] $C1m1(\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = \mathbf{a} + 2\mathbf{c}, \mathbf{c}' = 2\mathbf{c})(Cm, 8)$; [3] $C1m1(\mathbf{b}' = 3\mathbf{b})(Cm, 8)$

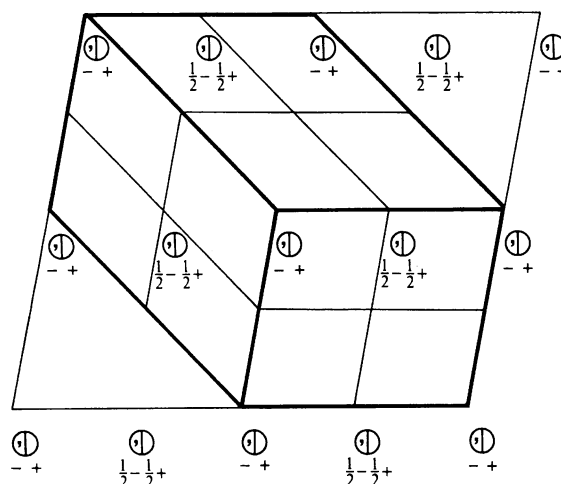
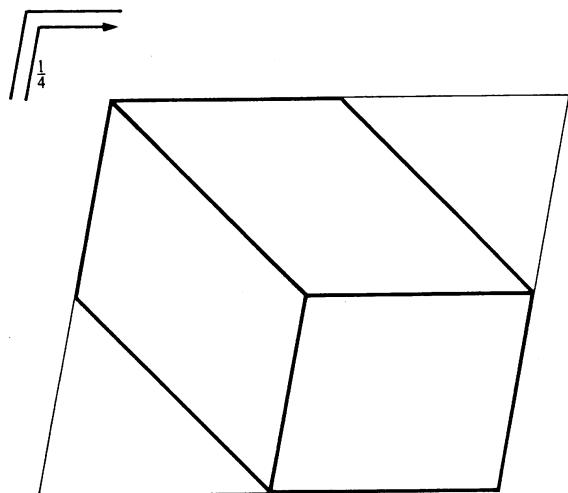
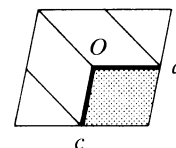
Minimal non-isomorphic supergroups

- I** [2] $C2/m(12)$; [2] $Cmm2(35)$; [2] $Cmc2, (36)$; [2] $Amm2(38)$; [2] $Aem2(39)$; [2] $Fmm2(42)$; [2] $Imm2(44)$; [2] $Ima2(46)$;
 [3] $P3m1(156)$; [3] $P31m(157)$; [3] $R3m(160)$
- II** [2] $P1m1(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b})(Pm, 6)$

Cm C_s^3 m

Monoclinic

No. 8

UNIQUE AXIS b , DIFFERENT CELL CHOICES $C1m1$ UNIQUE AXIS b , CELL CHOICE 1**Origin** on mirror plane m **Asymmetric unit** $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, 0) +$

4	b	1	(1) x, y, z	(2) x, \bar{y}, z
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Reflection conditions

General:

 hkl : $h + k = 2n$ $h0l$: $h = 2n$ $0kl$: $k = 2n$ $hk0$: $h + k = 2n$ $0k0$: $k = 2n$ $h00$: $h = 2n$

Special: no extra conditions

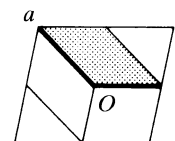
2	a	m	$x, 0, z$
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A 1 m 1UNIQUE AXIS *b*, CELL CHOICE 2**Origin** on mirror plane *m***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates
		$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

4	<i>b</i>	1	(1) x,y,z	(2) x,\bar{y},z
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2	<i>a</i>	<i>m</i>	$x,0,z$
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Reflection conditions

General:

$hkl : k + l = 2n$

$h0l : l = 2n$

$0kl : k + l = 2n$

$hk0 : k = 2n$

$0k0 : k = 2n$

$00l : l = 2n$

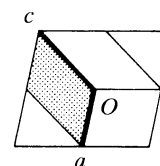
Special: no extra conditions

I 1 m 1UNIQUE AXIS *b*, CELL CHOICE 3**Origin** on mirror plane *m***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates
		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

4	<i>b</i>	1	(1) x,y,z	(2) x,\bar{y},z
---	----------	---	-------------	-------------------

2	<i>a</i>	<i>m</i>	$x,0,z$
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Reflection conditions

General:

$hkl : h + k + l = 2n$

$h0l : h + l = 2n$

$0kl : k + l = 2n$

$hk0 : h + k = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

$00l : l = 2n$

Special: no extra conditions

Cm

C_s^3

m

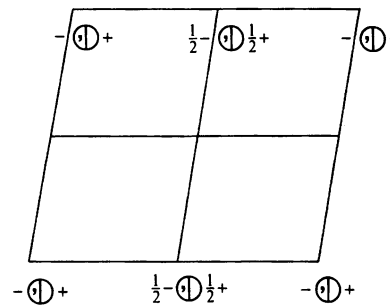
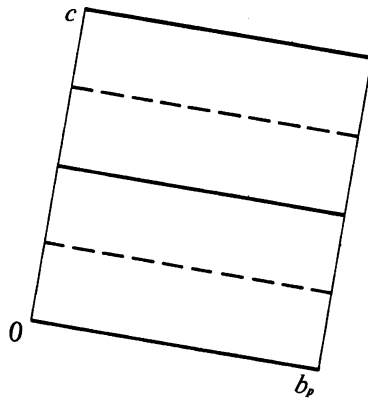
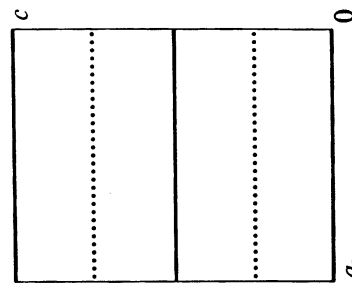
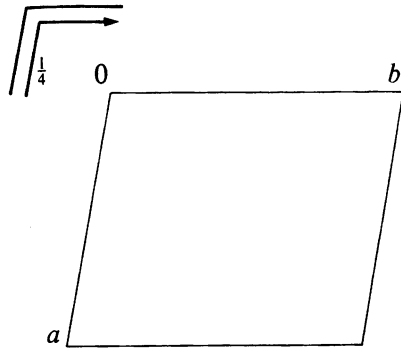
Monoclinic

No. 8

$A11m$

Patterson symmetry $A112/m$

UNIQUE AXIS c , CELL CHOICE 1



Origin on mirror plane m

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1
- (2) $m \ x,y,0$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) $t(0, \frac{1}{2}, \frac{1}{2})$
- (2) $b \ x,y, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	General:
4	<i>b</i> 1	(1) x,y,z	(2) x,y,\bar{z}	$hkl : k+l=2n$ $hk0 : k=2n$ $0kl : k+l=2n$ $h0l : l=2n$ $00l : l=2n$ $0k0 : k=2n$
2	<i>a</i> <i>m</i>	$x,y,0$		Special: no extra conditions

Symmetry of special projections

Along $[001]$ $p1$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0,0,z$

Along $[100]$ $c11m$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along $[010]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at $0,y,0$

Maximal non-isomorphic subgroups

- I** [2] $A1(P1, 1)$ 1+
- IIa** [2] $P11b(Pc, 7)$ 1; $2 + (0, \frac{1}{2}, \frac{1}{2})$
 [2] $P11m(Pm, 6)$ 1; 2
- IIb** [2] $A11a(\mathbf{a}' = 2\mathbf{a})(Cc, 9)$; [2] $I11a(\mathbf{a}' = 2\mathbf{a})(Cc, 9)$

Maximal isomorphic subgroups of lowest index

- IIc** [2] $A11m(\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})(Cm, 8)$; [3] $A11m(\mathbf{c}' = 3\mathbf{c})(Cm, 8)$

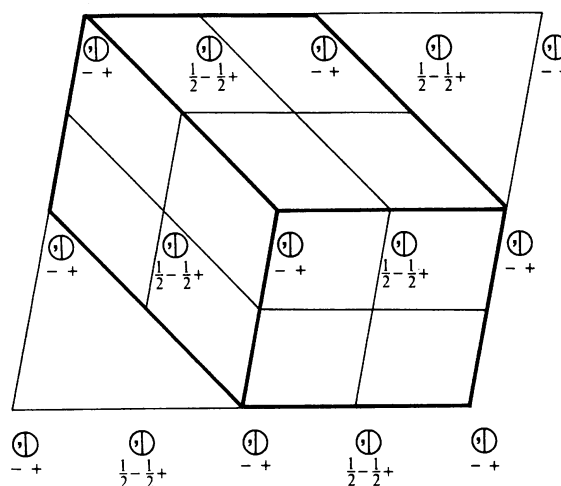
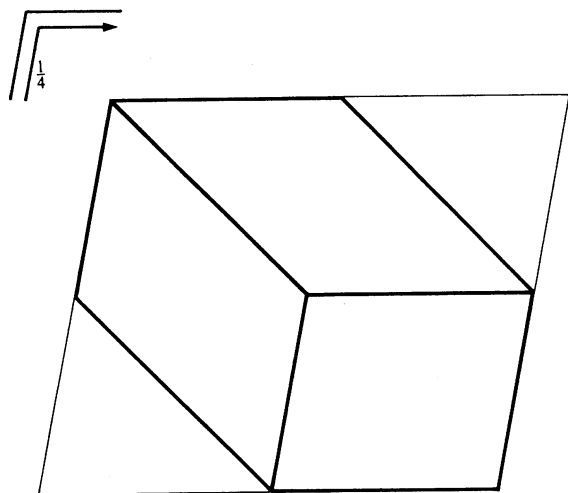
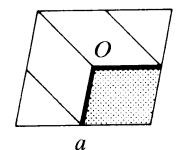
Minimal non-isomorphic supergroups

- I** [2] $C2/m(12)$; [2] $Cmm2(35)$; [2] $Cmc2_1(36)$; [2] $Amm2(38)$; [2] $Aem2(39)$; [2] $Fmm2(42)$; [2] $Imm2(44)$; [2] $Ima2(46)$;
 [3] $P3m1(156)$; [3] $P31m(157)$; [3] $R3m(160)$
- II** [2] $P11m(\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})(Pm, 6)$

Cm C_s^3 m

Monoclinic

No. 8

UNIQUE AXIS c , DIFFERENT CELL CHOICES $A11m$ UNIQUE AXIS c , CELL CHOICE 1**Origin** on mirror plane m **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (0, \frac{1}{2}, \frac{1}{2}) +$

4	b	1	(1) x, y, z	(2) x, y, \bar{z}
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Reflection conditions

General:

 $hkl : k + l = 2n$ $hk0 : k = 2n$ $0kl : k + l = 2n$ $h0l : l = 2n$ $00l : l = 2n$ $0k0 : k = 2n$

Special: no extra conditions

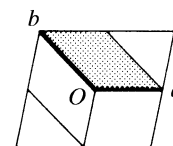
2	a	m	$x, y, 0$
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B11mUNIQUE AXIS c , CELL CHOICE 2**Origin** on mirror plane m **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates
		$(0,0,0)+ (\frac{1}{2},0,\frac{1}{2})+$

4	<i>b</i>	1	(1) x,y,z	(2) x,y,\bar{z}
---	----------	---	-------------	-------------------

2	<i>a</i>	<i>m</i>	$x,y,0$
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Reflection conditions

General:

$hkl : h + l = 2n$

$hk0 : h = 2n$

$0kl : l = 2n$

$h0l : h + l = 2n$

$00l : l = 2n$

$h00 : h = 2n$

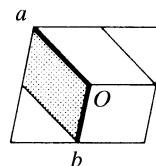
Special: no extra conditions

I11mUNIQUE AXIS c , CELL CHOICE 3**Origin** on mirror plane m **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

4	<i>b</i>	1	(1) x,y,z	(2) x,y,\bar{z}
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2	<i>a</i>	<i>m</i>	$x,y,0$
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Reflection conditions

General:

$hkl : h + k + l = 2n$

$hk0 : h + k = 2n$

$0kl : k + l = 2n$

$h0l : h + l = 2n$

$00l : l = 2n$

$h00 : h = 2n$

$0k0 : k = 2n$

Special: no extra conditions

Cc

C_s^4

m

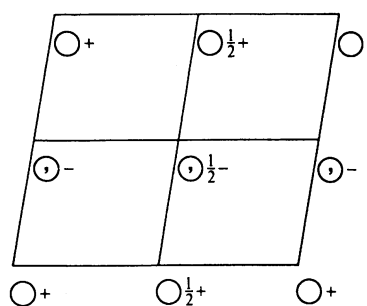
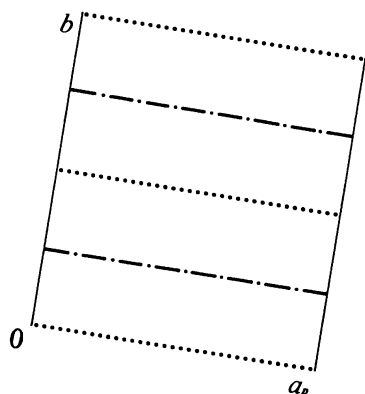
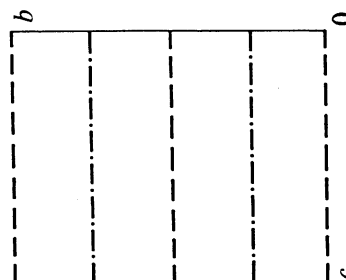
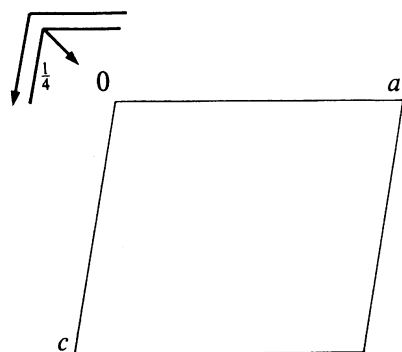
Monoclinic

No. 9

$C1c1$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $c \ x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $n(\frac{1}{2},0,\frac{1}{2}) \ x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$	General:
4 <i>a</i> 1	(1) x,y,z (2) $x,\bar{y},z+\frac{1}{2}$	$hkl : h+k=2n$ $h0l : h,l=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$ $00l : l=2n$

Symmetry of special projections

Along [001] $c11m$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

- I** [2] $C1 (P1, 1)$ 1+
IIa [2] $P1c1 (Pc, 7)$ 1; 2
[2] $P1n1 (Pc, 7)$ 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$
IIb none

Maximal isomorphic subgroups of lowest index

- IIc** [3] $C1c1 (\mathbf{b}' = 3\mathbf{b}) (Cc, 9)$; [3] $C1c1 (\mathbf{c}' = 3\mathbf{c}) (Cc, 9)$; [3] $C1c1 (\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$ or $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = \mathbf{a} + \mathbf{c}) (Cc, 9)$

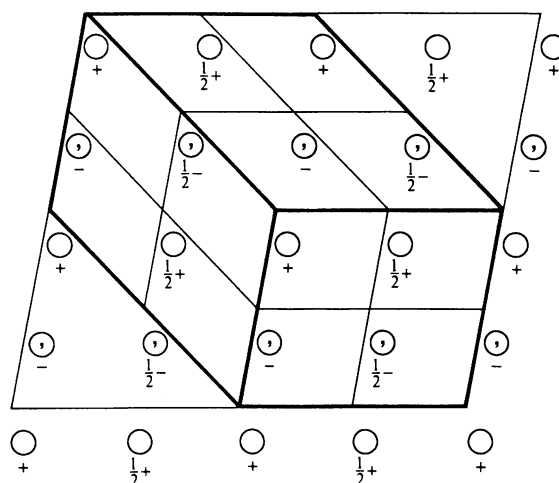
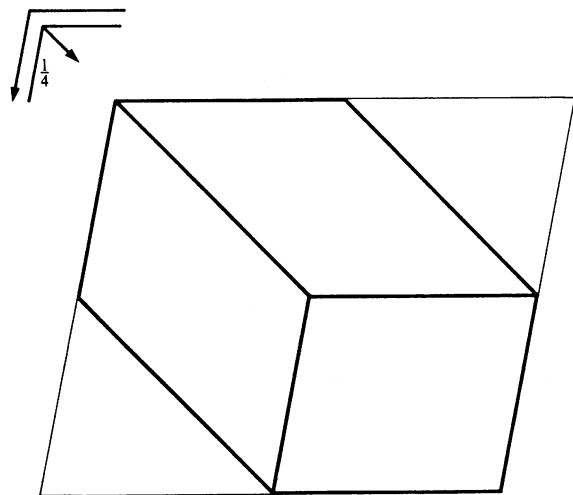
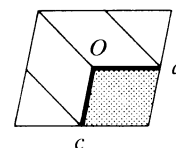
Minimal non-isomorphic supergroups

- I** [2] $C2/c (15)$; [2] $Cmc2_1 (36)$; [2] $Ccc2 (37)$; [2] $Ama2 (40)$; [2] $Aea2 (41)$; [2] $Fdd2 (43)$; [2] $Iba2 (45)$; [2] $Ima2 (46)$;
[3] $P3c1 (158)$; [3] $P31c (159)$; [3] $R3c (161)$
II [2] $Fm1 (Cm, 8)$; [2] $C1m1 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (Cm, 8)$; [2] $P1c1 (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}) (Pc, 7)$

Cc C_s^4 m

Monoclinic

No. 9

UNIQUE AXIS b , DIFFERENT CELL CHOICES $C1c1$ UNIQUE AXIS b , CELL CHOICE 1**Origin** on glide plane c **Asymmetric unit** $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

4	a	1	(1) x, y, z	(2) $x, \bar{y}, z + \frac{1}{2}$
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Reflection conditions

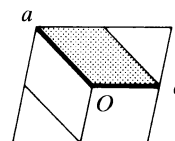
General:

 hkl : $h + k = 2n$ $h0l$: $h, l = 2n$ $0kl$: $k = 2n$ $hk0$: $h + k = 2n$ $0k0$: $k = 2n$ $h00$: $h = 2n$ $00l$: $l = 2n$

A1n1UNIQUE AXIS *b*, CELL CHOICE 2**Origin** on glide plane *n***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (0, \frac{1}{2}, \frac{1}{2}) +$

4	<i>a</i>	1	(1) x, y, z	(2) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$
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Reflection conditions

General:

$$hkl : k + l = 2n$$

$$h0l : h, l = 2n$$

$$0kl : k + l = 2n$$

$$hk0 : k = 2n$$

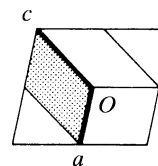
$$0k0 : k = 2n$$

$$h00 : h = 2n$$

$$00l : l = 2n$$
I1a1UNIQUE AXIS *b*, CELL CHOICE 3**Origin** on glide plane *a***Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$

4	<i>a</i>	1	(1) x, y, z	(2) $x + \frac{1}{2}, \bar{y}, z$
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Reflection conditions

General:

$$hkl : h + k + l = 2n$$

$$h0l : h, l = 2n$$

$$0kl : k + l = 2n$$

$$hk0 : h + k = 2n$$

$$0k0 : k = 2n$$

$$h00 : h = 2n$$

$$00l : l = 2n$$

Cc

No. 9

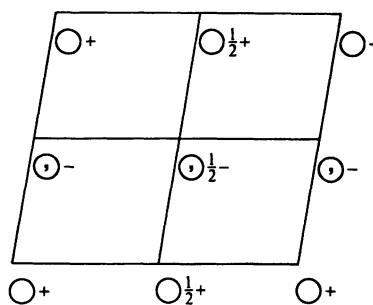
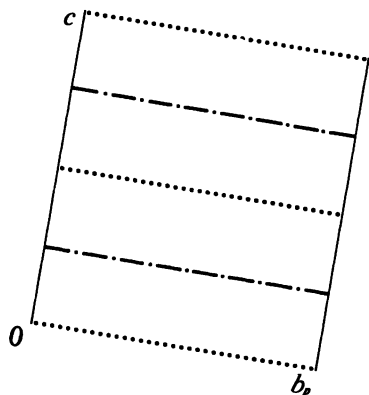
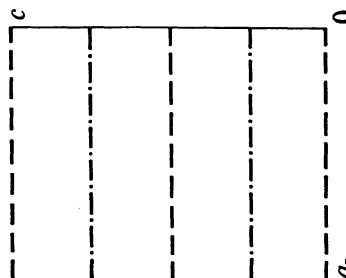
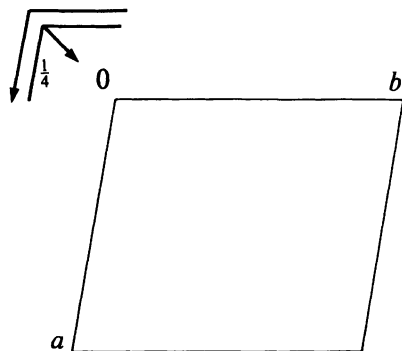
 C_s^4

A11a

 m

Monoclinic

Patterson symmetry A112/m

UNIQUE AXIS c , CELL CHOICE 1**Origin** on glide plane a **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Symmetry operations**For $(0,0,0)+$ set(1) 1 (2) a $x, y, 0$ For $(0, \frac{1}{2}, \frac{1}{2})+$ set(1) $t(0, \frac{1}{2}, \frac{1}{2})$ (2) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
		$(0,0,0)+$	General:
		$(0, \frac{1}{2}, \frac{1}{2})+$	$hkl : k+l=2n$
4	<i>a</i> 1	(1) x,y,z	$hk0 : h,k=2n$
		(2) $x+\frac{1}{2},y,\bar{z}$	$0kl : k+l=2n$
			$h0l : l=2n$
			$00l : l=2n$
			$h00 : h=2n$
			$0k0 : k=2n$

Symmetry of special projections

Along $[001]$ $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ Origin at $0,0,z$	Along $[100]$ $c11m$ $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$	Along $[010]$ $p1g1$ $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$ Origin at $0,y,0$
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Maximal non-isomorphic subgroups

I	$[2]A1(P1, 1)$	$1+$
IIa	$[2]P11a(Pc, 7)$	$1; 2$
	$[2]P11n(Pc, 7)$	$1; 2 + (0, \frac{1}{2}, \frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc $[3]A11a(\mathbf{c}' = 3\mathbf{c})(Cc, 9)$; $[3]A11a(\mathbf{a}' = 3\mathbf{a})(Cc, 9)$; $[3]A11a(\mathbf{b}' = 3\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = 3\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = 3\mathbf{b})(Cc, 9)$

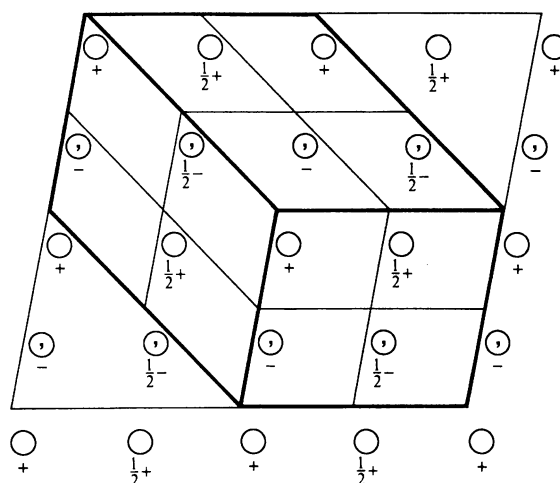
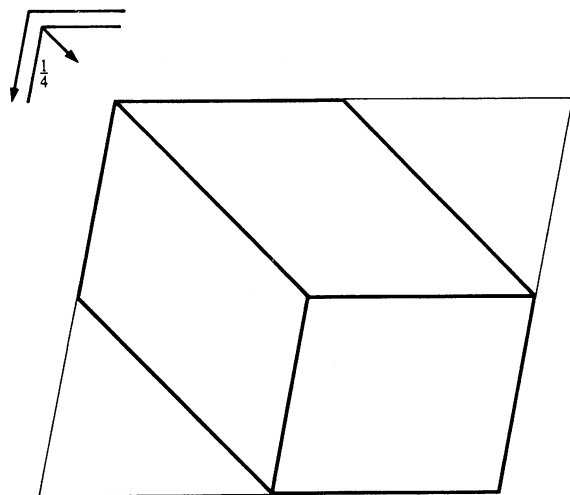
Minimal non-isomorphic supergroups

I	$[2]C2/c(15)$; $[2]Cmc2_1(36)$; $[2]Ccc2(37)$; $[2]Ama2(40)$; $[2]Aea2(41)$; $[2]Fdd2(43)$; $[2]Iba2(45)$; $[2]Ima2(46)$; $[3]P3c1(158)$; $[3]P31c(159)$; $[3]R3c(161)$
II	$[2]F11m(Cm, 8)$; $[2]A11m(\mathbf{a}' = \frac{1}{2}\mathbf{a})(Cm, 8)$; $[2]P11a(\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})(Pc, 7)$

Cc C_s^4 m

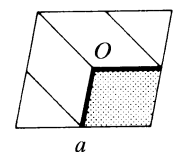
Monoclinic

No. 9

UNIQUE AXIS c , DIFFERENT CELL CHOICES $A11a$ UNIQUE AXIS c , CELL CHOICE 1**Origin** on glide plane a **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

4	a	1	(1) x,y,z	(2) $x + \frac{1}{2}, y, \bar{z}$
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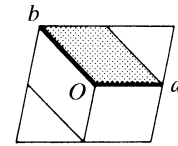
Reflection conditions

General:

 $hkl : k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $h0l : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$

B11nUNIQUE AXIS c , CELL CHOICE 2**Origin** on glide plane n **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},0,\frac{1}{2}) +$
4 a 1	(1) x,y,z (2) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$



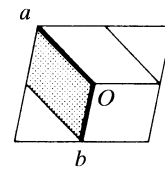
Reflection conditions

General:

$$\begin{aligned}
 hkl &: h + l = 2n \\
 hk0 &: h, k = 2n \\
 0kl &: l = 2n \\
 h0l &: h + l = 2n \\
 00l &: l = 2n \\
 h00 &: h = 2n \\
 0k0 &: k = 2n
 \end{aligned}$$

I11bUNIQUE AXIS c , CELL CHOICE 3**Origin** on glide plane b **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$
4 a 1	(1) x,y,z (2) $x,y + \frac{1}{2}, \bar{z}$



Reflection conditions

General:

$$\begin{aligned}
 hkl &: h + k + l = 2n \\
 hk0 &: h, k = 2n \\
 0kl &: k + l = 2n \\
 h0l &: h + l = 2n \\
 00l &: l = 2n \\
 h00 &: h = 2n \\
 0k0 &: k = 2n
 \end{aligned}$$

$P2/m$

C_{2h}^1

$2/m$

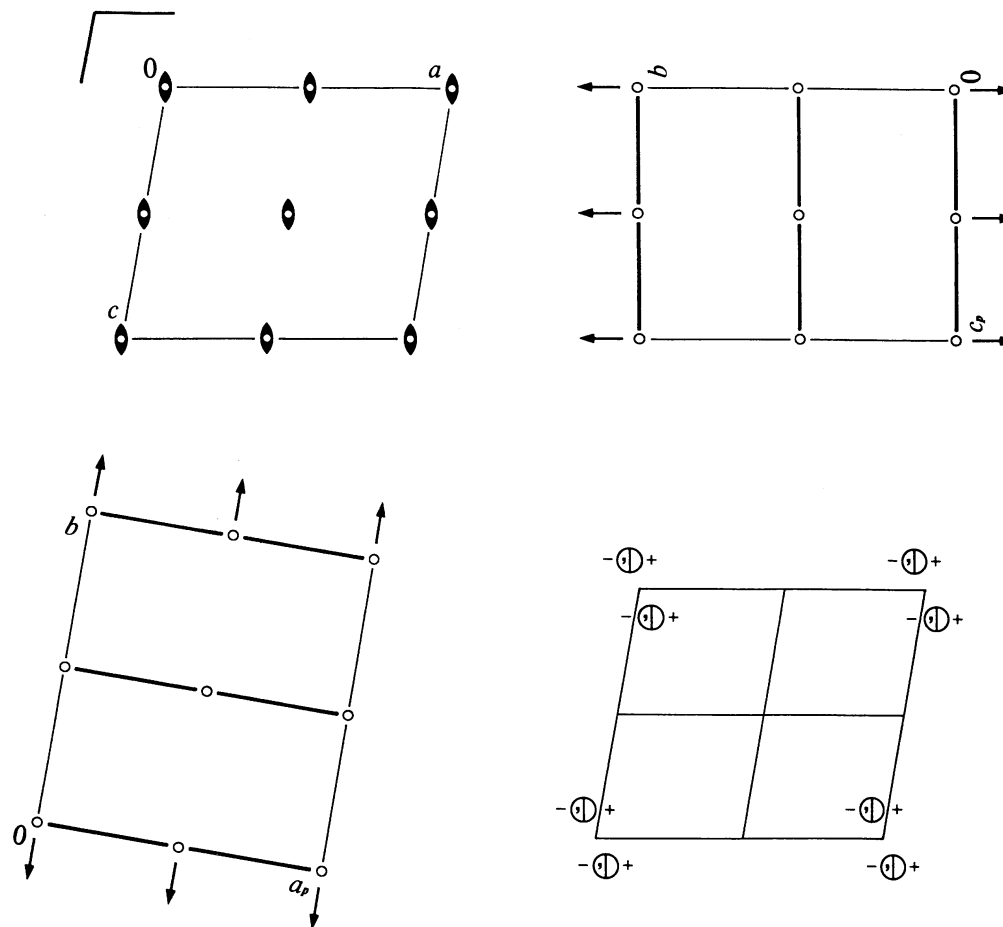
Monoclinic

No. 10

$P12/m1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin at centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2 \ 0,y,0$ (3) $\bar{1} \ 0,0,0$ (4) $m \ x,0,z$

Maximal isomorphic subgroups of lowest index

IIc $[2] P12/m1 (b' = 2b) (P2/m, 10); [2] P12/m1 (c' = 2c \text{ or } a' = 2a \text{ or } a' = a + c, c' = -a + c) (P2/m, 10)$

Minimal non-isomorphic supergroups

I $[2] Pmmm (47); [2] Pccm (49); [2] Pmma (51); [2] Pmna (53); [2] Pbam (55); [2] Pnmm (58); [2] Cmmm (65); [2] Cccm (66); [2] P4/m (83); [2] P4_2/m (84); [3] P6/m (175)$

II $[2] C12/m1 (C2/m, 12); [2] A12/m1 (C2/m, 12); [2] I12/m1 (C2/m, 12)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
4	<i>o</i> 1	(1) x, y, z	(2) \bar{x}, y, \bar{z}	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, \bar{y}, z	General: no conditions Special: no extra conditions
2	<i>n</i> <i>m</i>	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, \bar{z}$			
2	<i>m</i> <i>m</i>	$x, 0, z$	$\bar{x}, 0, \bar{z}$			
2	<i>l</i> 2	$\frac{1}{2}, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$			
2	<i>k</i> 2	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$			
2	<i>j</i> 2	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$			
2	<i>i</i> 2	$0, y, 0$	$0, \bar{y}, 0$			
1	<i>h</i> $2/m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				
1	<i>g</i> $2/m$	$\frac{1}{2}, 0, \frac{1}{2}$				
1	<i>f</i> $2/m$	$0, \frac{1}{2}, \frac{1}{2}$				
1	<i>e</i> $2/m$	$\frac{1}{2}, \frac{1}{2}, 0$				
1	<i>d</i> $2/m$	$\frac{1}{2}, 0, 0$				
1	<i>c</i> $2/m$	$0, 0, \frac{1}{2}$				
1	<i>b</i> $2/m$	$0, \frac{1}{2}, 0$				
1	<i>a</i> $2/m$	$0, 0, 0$				

Symmetry of special projections

Along [001] $p2mm$

$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$

Origin at $x, 0, 0$

Along [010] $p2$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm , 6) 1; 4
 [2] $P121$ ($P2$, 3) 1; 2
 [2] $P\bar{1}$ (2) 1; 3

IIa none

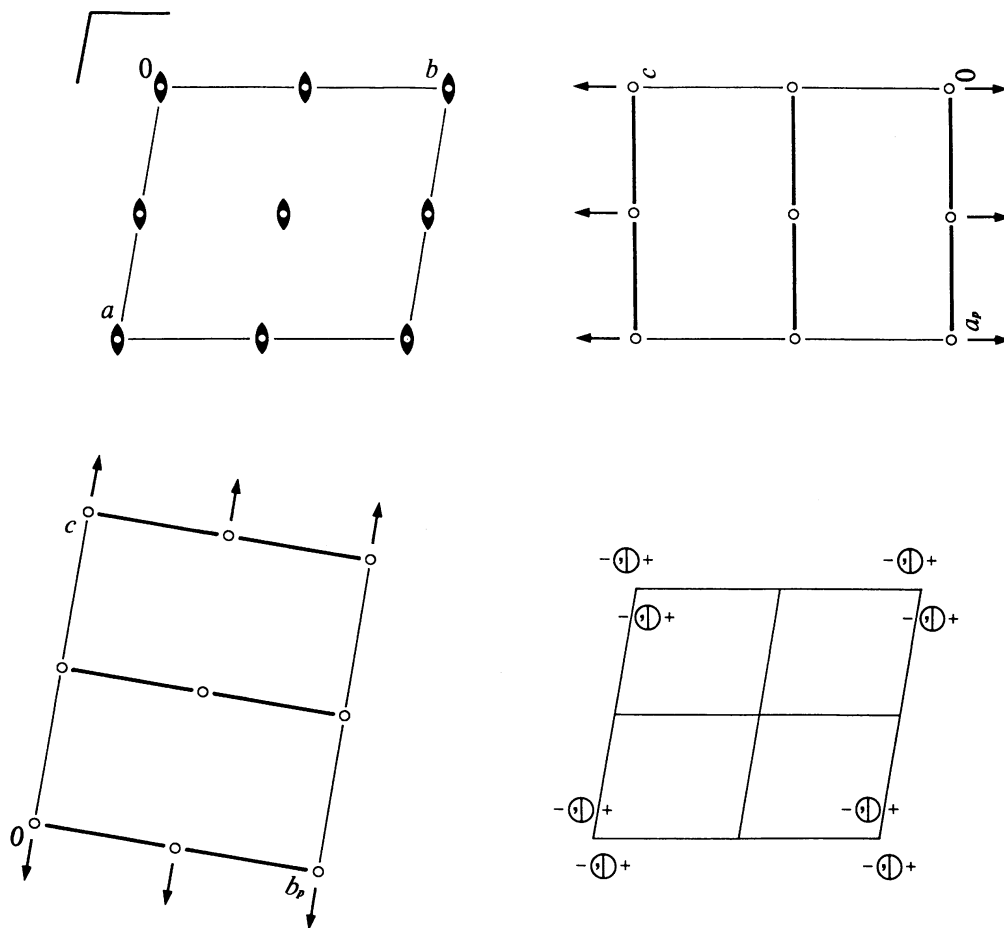
IIb [2] $P12_1/m1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $P12/a1$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13);
 [2] $B12/e1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $C12/m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($C2/m$, 12); [2] $A12/m1$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12);
 [2] $F12/m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

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$P2/m$ C_{2h}^1 $2/m$

Monoclinic

No. 10

 $P112/m$ Patterson symmetry $P112/m$ UNIQUE AXIS c **Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$ **Symmetry operations**(1) 1 (2) 2 $0,0,z$ (3) $\bar{1}$ $0,0,0$ (4) m $x,y,0$ **Maximal isomorphic subgroups of lowest index****IIc** $[2] P112/m$ ($c' = 2c$) ($P2/m, 10$); $[2] P112/m$ ($a' = 2a$ or $b' = 2b$ or $a' = a - b, b' = a + b$) ($P2/m, 10$)**Minimal non-isomorphic supergroups****I** $[2] Pmmm$ (47); $[2] Pccm$ (49); $[2] Pmma$ (51); $[2] Pmna$ (53); $[2] Pbam$ (55); $[2] Pnnm$ (58); $[2] Cmmm$ (65); $[2] Cccm$ (66); $[2] P4/m$ (83); $[2] P4_2/m$ (84); $[3] P6/m$ (175)**II** $[2] A112/m$ ($C2/m, 12$); $[2] B112/m$ ($C2/m, 12$); $[2] I112/m$ ($C2/m, 12$)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>o</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, y, \bar{z}	General: no conditions Special: no extra conditions
2 <i>n</i> <i>m</i>	$x, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$			
2 <i>m</i> <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$			
2 <i>l</i> 2	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			
2 <i>k</i> 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$			
2 <i>j</i> 2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$			
2 <i>i</i> 2	$0, 0, z$	$0, 0, \bar{z}$			
1 <i>h</i> $2/m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				
1 <i>g</i> $2/m$	$\frac{1}{2}, \frac{1}{2}, 0$				
1 <i>f</i> $2/m$	$\frac{1}{2}, 0, \frac{1}{2}$				
1 <i>e</i> $2/m$	$0, \frac{1}{2}, \frac{1}{2}$				
1 <i>d</i> $2/m$	$0, \frac{1}{2}, 0$				
1 <i>c</i> $2/m$	$\frac{1}{2}, 0, 0$				
1 <i>b</i> $2/m$	$0, 0, \frac{1}{2}$				
1 <i>a</i> $2/m$	$0, 0, 0$				

Symmetry of special projections

Along [001] $p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I [2] $P11m$ (Pm , 6) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2
 [2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P112/m$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1/m$, 11); [2] $P112/a$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13); [2] $P112/b$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13);
 [2] $C112/e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $A112/m$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $B112/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12);
 [2] $F112/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

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$P2_1/m$

C_{2h}^2

$2/m$

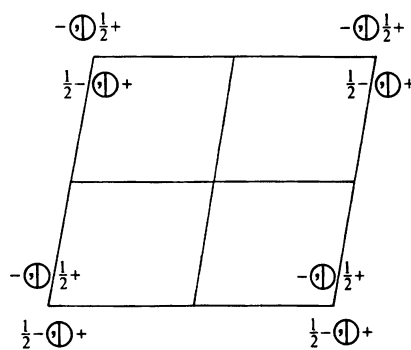
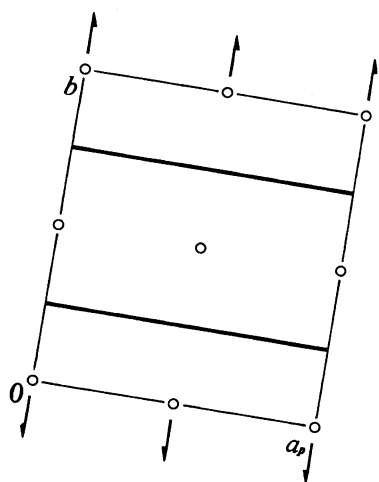
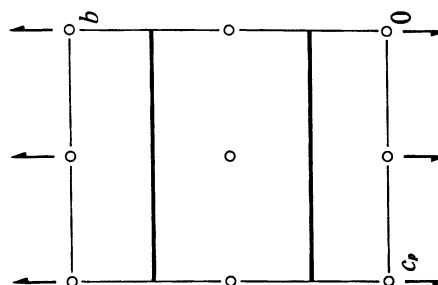
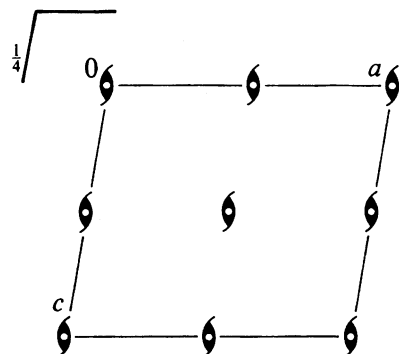
Monoclinic

No. 11

$P12_1/m1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin at $\bar{1}$ on 2_1

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, \frac{1}{2}, 0) \ 0, y, 0$ (3) $\bar{1} \ 0, 0, 0$ (4) $m \ x, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>f</i> 1	(1) x, y, z	(2) $\bar{x}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y} + \frac{1}{2}, z$	General: $0k0 : k = 2n$ Special: as above, plus no extra conditions
2 <i>e</i> m	$x, \frac{1}{4}, z$	$\bar{x}, \frac{3}{4}, \bar{z}$			$hkl : k = 2n$
2 <i>d</i> $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : k = 2n$
2 <i>c</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : k = 2n$
2 <i>b</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : k = 2n$
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, 0$			$hkl : k = 2n$

Symmetry of special projections

Along $[001]$ $p2gm$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x, 0, 0$

Along $[010]$ $p2$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I $[2] P1m1 (Pm, 6)$ 1; 4
 $[2] P12_11 (P2_1, 4)$ 1; 2
 $[2] P\bar{1} (2)$ 1; 3

IIa none

IIb $[2] P12_1/c1 (\mathbf{c}' = 2\mathbf{c}) (P2_1/c, 14)$; $[2] P12_1/a1 (\mathbf{a}' = 2\mathbf{a}) (P2_1/c, 14)$; $[2] B12_1/e1 (\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}) (P2_1/c, 14)$

Maximal isomorphic subgroups of lowest index

IIc $[2] P12_1/m1 (\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}) (P2_1/m, 11)$; $[3] P12_1/m1 (\mathbf{b}' = 3\mathbf{b}) (P2_1/m, 11)$

Minimal non-isomorphic supergroups

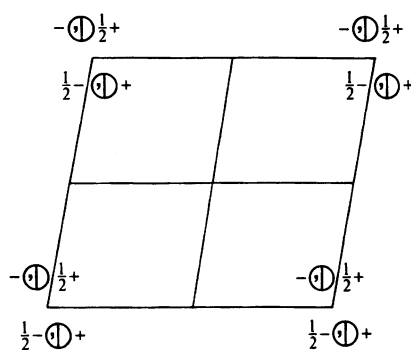
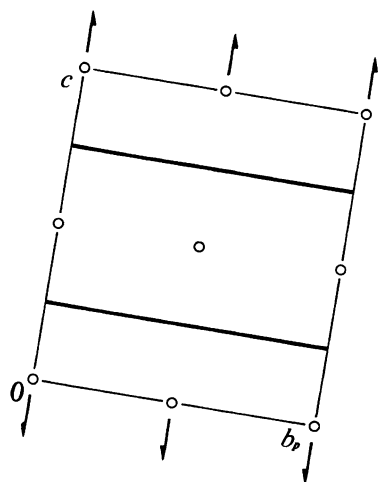
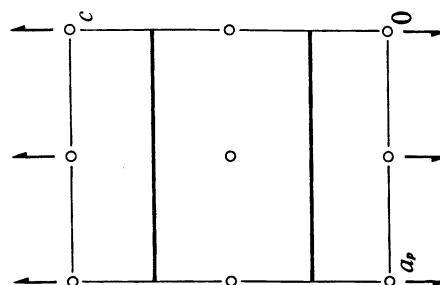
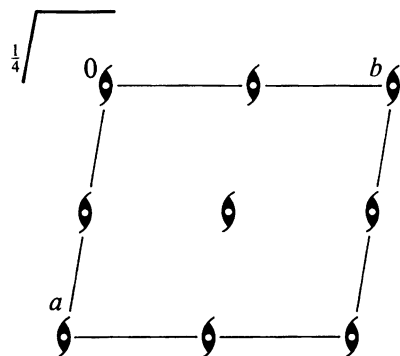
I $[2] Pmma (51)$; $[2] Pbcm (57)$; $[2] Pmnm (59)$; $[2] Pnma (62)$; $[2] Cmcm (63)$; $[3] P6_3/m (176)$

II $[2] C12/m1 (C2/m, 12)$; $[2] A12/m1 (C2/m, 12)$; $[2] I12/m1 (C2/m, 12)$; $[2] P12/m1 (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (P2/m, 10)$

$P2_1/m$ C_{2h}^2 $2/m$

Monoclinic

No. 11

 $P112_1/m$ Patterson symmetry $P112/m$ UNIQUE AXIS c Origin at $\bar{1}$ on 2_1 Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

(1) 1 (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (3) $\bar{1}$ $0, 0, 0$ (4) m $x, y, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>f</i> 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) \bar{x},\bar{y},\bar{z}	(4) $x,y,\bar{z}+\frac{1}{2}$	General: $00l : l = 2n$ Special: as above, plus no extra conditions
2 <i>e</i> m	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$			$hkl : l = 2n$
2 <i>d</i> $\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl : l = 2n$
2 <i>c</i> $\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			$hkl : l = 2n$
2 <i>b</i> $\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : l = 2n$
2 <i>a</i> $\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along $[001] p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along $[100] p2gm$
 $\mathbf{a}' = \mathbf{b}'_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along $[010] p2mg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}'_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I $[2] P11m (Pm, 6)$ 1; 4
 $[2] P112_1 (P2_1, 4)$ 1; 2
 $[2] P\bar{1} (2)$ 1; 3

IIa none

IIb $[2] P112_1/a (\mathbf{a}' = 2\mathbf{a}) (P2_1/c, 14)$; $[2] P112_1/b (\mathbf{b}' = 2\mathbf{b}) (P2_1/c, 14)$; $[2] C112_1/e (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P2_1/c, 14)$

Maximal isomorphic subgroups of lowest index

IIc $[2] P112_1/m (\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}) (P2_1/m, 11)$; $[3] P112_1/m (\mathbf{c}' = 3\mathbf{c}) (P2_1/m, 11)$

Minimal non-isomorphic supergroups

I $[2] Pmma (51)$; $[2] Pbcm (57)$; $[2] Pmnm (59)$; $[2] Pnma (62)$; $[2] Cmcm (63)$; $[3] P6_3/m (176)$

II $[2] A112/m (C2/m, 12)$; $[2] B112/m (C2/m, 12)$; $[2] I112/m (C2/m, 12)$; $[2] P112/m (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2/m, 10)$

$C2/m$

C_{2h}^3

$2/m$

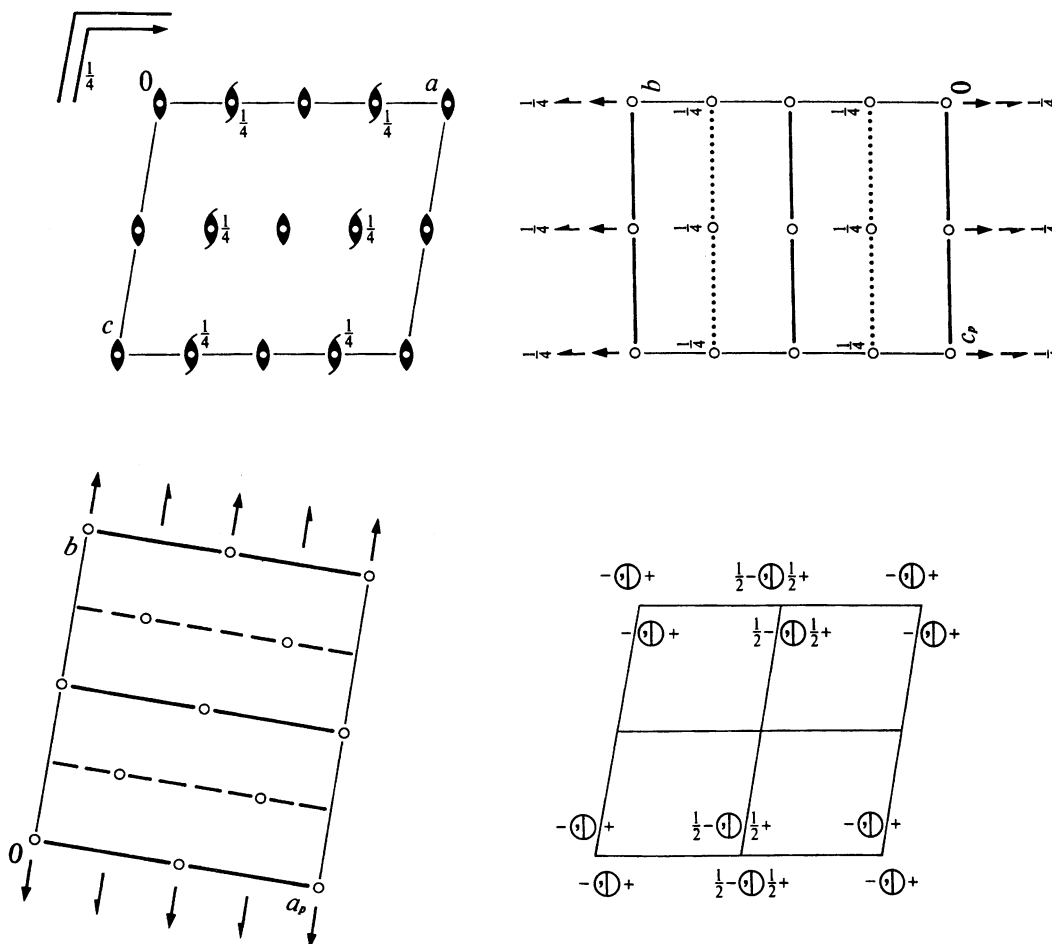
Monoclinic

No. 12

$C12/m1$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-------|-----------------|-----------------------|-----------------|
| (1) 1 | (2) $2 \ 0,y,0$ | (3) $\bar{1} \ 0,0,0$ | (4) $m \ x,0,z$ |
|-------|-----------------|-----------------------|-----------------|

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|--------------------------------------|--|---|-----------------------------|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$ | (3) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, 0$ | (4) $a \ x, \frac{1}{4}, z$ |
|--------------------------------------|--|---|-----------------------------|

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+ $(\frac{1}{2},\frac{1}{2},0)$ +				General:
8 <i>j</i> 1	(1) x,y,z	(2) \bar{x},y,\bar{z}	(3) \bar{x},\bar{y},\bar{z}	(4) x,\bar{y},z	$hkl : h+k=2n$ $h0l : h=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$
4 <i>i</i> <i>m</i>	$x,0,z$	$\bar{x},0,\bar{z}$			Special: as above, plus no extra conditions
4 <i>h</i> 2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4 <i>g</i> 2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4 <i>f</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : h=2n$
4 <i>e</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			$hkl : h=2n$
2 <i>d</i> $2/m$	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2 <i>c</i> $2/m$	$0,0,\frac{1}{2}$				no extra conditions
2 <i>b</i> $2/m$	$0,\frac{1}{2},0$				no extra conditions
2 <i>a</i> $2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at $x,0,0$

Along [010] $p2$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C1m1$ (Cm , 8)	(1; 4)+
	[2] $C121$ ($C2$, 5)	(1; 2)+
	[2] $C\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P12_1/a1$ ($P2_1/c$, 14)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12/a1$ ($P2/c$, 13)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12_1/m1$ ($P2_1/m$, 11)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12/m1$ ($P2/m$, 10)	1; 2; 3; 4
IIb	[2] $C12/c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($C2/c$, 15); [2] $I12/c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($C2/c$, 15)	

Maximal isomorphic subgroups of lowest index

IIc [2] $C12/m1$ ($\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = \mathbf{a} + 2\mathbf{c}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [3] $C12/m1$ ($\mathbf{b}' = 3\mathbf{b}$) ($C2/m$, 12)

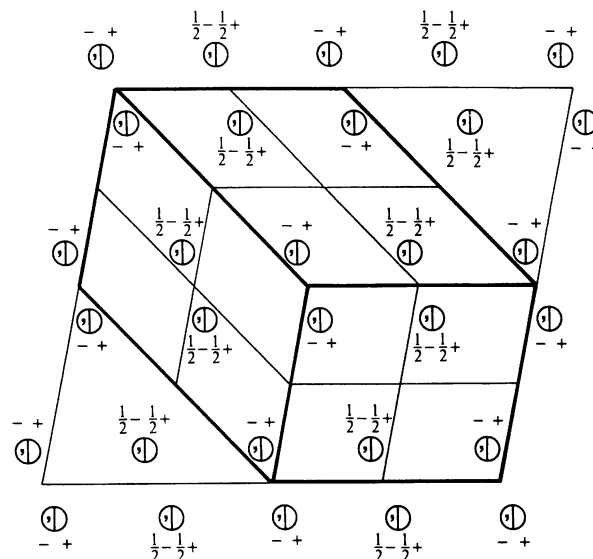
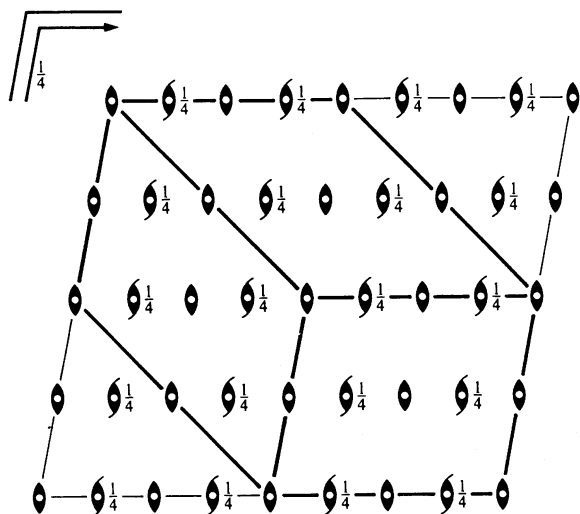
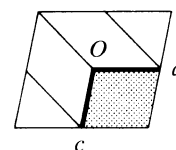
Minimal non-isomorphic supergroups

I	[2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $Fmmm$ (69); [2] $Immm$ (71); [2] $Ibam$ (72); [2] $Imma$ (74); [2] $I4/m$ (87); [3] $P\bar{3}1m$ (162); [3] $P\bar{3}m1$ (164); [3] $R\bar{3}m$ (166)
II	[2] $P12/m1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P2/m$, 10)

$C2/m$ C_{2h}^3 $2/m$

Monoclinic

No. 12

UNIQUE AXIS b , DIFFERENT CELL CHOICES $C12/m1$ UNIQUE AXIS b , CELL CHOICE 1Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$ 8 j 1 (1) x, y, z (2) \bar{x}, y, \bar{z} (3) $\bar{x}, \bar{y}, \bar{z}$ (4) x, \bar{y}, z

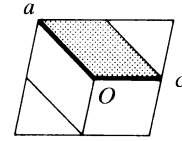
Reflection conditions

General:

 $hkl : h + k = 2n$ $hk0 : h + k = 2n$
 $h0l : h = 2n$ $0k0 : k = 2n$
 $0kl : k = 2n$ $h00 : h = 2n$

Special: as above, plus

4	i	m	$x, 0, z$	$\bar{x}, 0, \bar{z}$					no extra conditions	
4	h	2	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$	4	g	2	$0, y, 0$	$0, \bar{y}, 0$	no extra conditions
4	f	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	4	e	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h = 2n$
2	d	$2/m$	$0, \frac{1}{2}, \frac{1}{2}$		2	c	$2/m$	$0, 0, \frac{1}{2}$		no extra conditions
2	b	$2/m$	$0, \frac{1}{2}, 0$		2	a	$2/m$	$0, 0, 0$		no extra conditions

$A12/m1$ UNIQUE AXIS b , CELL CHOICE 2Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

Multiplicity	Wyckoff letter	Site symmetry	(1) x, y, z	(2) \bar{x}, y, \bar{z}	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, \bar{y}, z
8	j	1	x, y, z	\bar{x}, y, \bar{z}	$\bar{x}, \bar{y}, \bar{z}$	x, \bar{y}, z
4	i	m	$x, 0, z$	$\bar{x}, 0, \bar{z}$		
4	h	2	$\frac{1}{2}, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	4 g 2	$0, y, 0$ $0, \bar{y}, 0$
4	f	$\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	4 e $\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$ $0, \frac{1}{4}, \frac{3}{4}$
2	d	$2/m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		2 c $2/m$	$\frac{1}{2}, 0, \frac{1}{2}$
2	b	$2/m$	$0, \frac{1}{2}, 0$		2 a $2/m$	$0, 0, 0$

Reflection conditions

General:

$$\begin{aligned} hkl &: k+l=2n & hk0 &: k=2n \\ h0l &: l=2n & 0k0 &: k=2n \\ 0kl &: k+l=2n & 00l &: l=2n \end{aligned}$$

Special: as above, plus

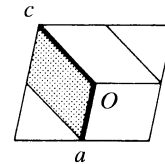
no extra conditions

no extra conditions

 $hkl : k=2n$

no extra conditions

no extra conditions

 $I12/m1$ UNIQUE AXIS b , CELL CHOICE 3Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

Multiplicity	Wyckoff letter	Site symmetry	(1) x, y, z	(2) \bar{x}, y, \bar{z}	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, \bar{y}, z
8	j	1	x, y, z	\bar{x}, y, \bar{z}	$\bar{x}, \bar{y}, \bar{z}$	x, \bar{y}, z
4	i	m	$x, 0, z$	$\bar{x}, 0, \bar{z}$		
4	h	2	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	4 g 2	$0, y, 0$ $0, \bar{y}, 0$
4	f	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	4 e $\bar{1}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
2	d	$2/m$	$\frac{1}{2}, \frac{1}{2}, 0$		2 c $2/m$	$\frac{1}{2}, 0, 0$
2	b	$2/m$	$0, \frac{1}{2}, 0$		2 a $2/m$	$0, 0, 0$

Reflection conditions

General:

$$\begin{aligned} hkl &: h+k+l=2n & 0k0 &: k=2n \\ h0l &: h+l=2n & h00 &: h=2n \\ 0kl &: k+l=2n & 00l &: l=2n \\ hk0 &: h+k=2n & & \end{aligned}$$

Special: as above, plus

no extra conditions

no extra conditions

 $hkl : k=2n$

no extra conditions

no extra conditions

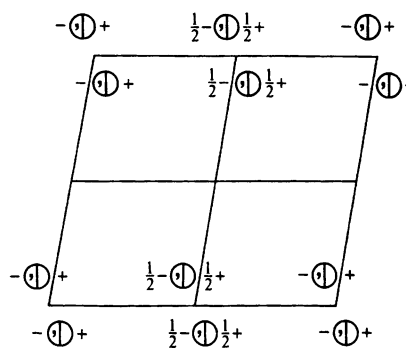
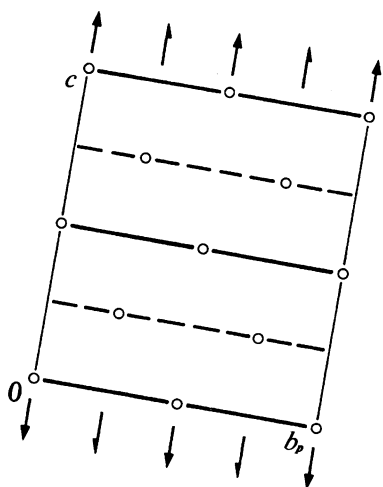
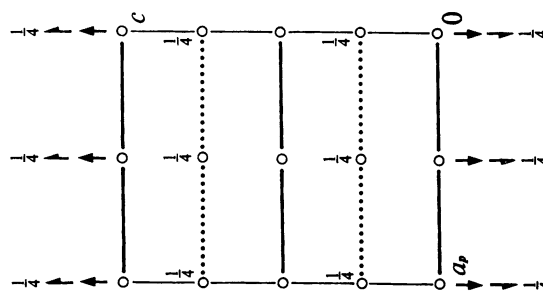
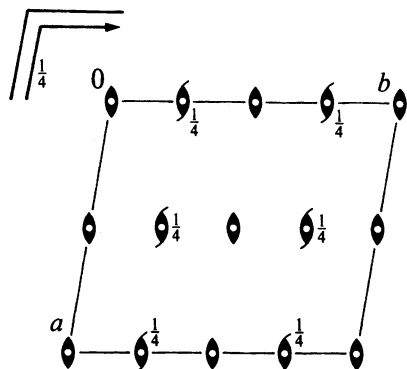
$C2/m$ C_{2h}^3 $2/m$

Monoclinic

No. 12

A112/m

Patterson symmetry A112/m

UNIQUE AXIS c , CELL CHOICE 1**Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$ **Symmetry operations**For $(0,0,0)+$ set

- | | | | |
|-------|-----------------|-----------------------|-----------------|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $\bar{1} \ 0,0,0$ | (4) $m \ x,y,0$ |
|-------|-----------------|-----------------------|-----------------|

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--------------------------------------|---|---|----------------------------|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0, \frac{1}{2}) \ 0, \frac{1}{4}, z$ | (3) $\bar{1} \ 0, \frac{1}{4}, \frac{1}{4}$ | (4) $b \ x,y, \frac{1}{4}$ |
|--------------------------------------|---|---|----------------------------|

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+			General:
8 <i>j</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) x, y, \bar{z}	$hkl : k + l = 2n$ $hk0 : k = 2n$ $0kl : k + l = 2n$ $h0l : l = 2n$ $00l : l = 2n$ $0k0 : k = 2n$
4 <i>i</i> <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$			Special: as above, plus no extra conditions
4 <i>h</i> 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
4 <i>g</i> 2	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
4 <i>f</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$			$hkl : k = 2n$
4 <i>e</i> $\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$			$hkl : k = 2n$
2 <i>d</i> 2/m	$\frac{1}{2}, 0, \frac{1}{2}$				no extra conditions
2 <i>c</i> 2/m	$\frac{1}{2}, 0, 0$				no extra conditions
2 <i>b</i> 2/m	$0, 0, \frac{1}{2}$				no extra conditions
2 <i>a</i> 2/m	$0, 0, 0$				no extra conditions

Symmetry of special projections

Along [001] $p2$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0, 0, z

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, 0, 0

Along [010] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at 0, y, 0

Maximal non-isomorphic subgroups

I	[2] $A11m$ (Cm , 8)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
	[2] $A\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P112_1/b$ ($P2_1/c$, 14)	1; 3; (2; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $P112/b$ ($P2/c$, 13)	1; 2; (3; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $P112_1/m$ ($P2_1/m$, 11)	1; 4; (2; 3) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 3; 4
IIb	[2] $A112/a$ ($\mathbf{a}' = 2\mathbf{a}$) ($C2/c$, 15); [2] $I112/a$ ($\mathbf{a}' = 2\mathbf{a}$) ($C2/c$, 15)	

Maximal isomorphic subgroups of lowest index

IIc [2] $A112/m$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) ($C2/m$, 12); [3] $A112/m$ ($\mathbf{c}' = 3\mathbf{c}$) ($C2/m$, 12)

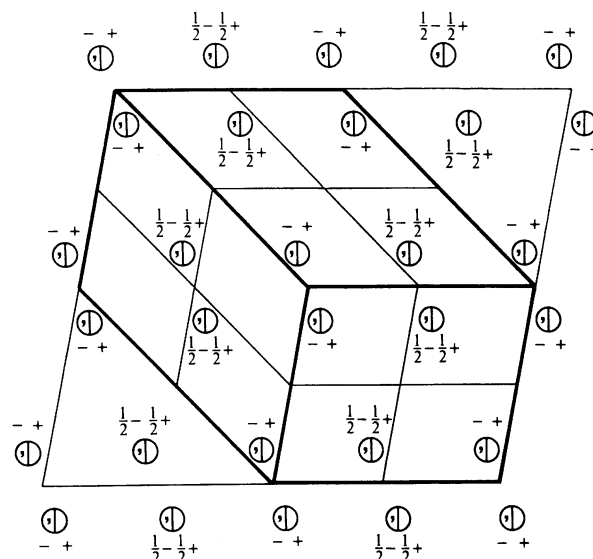
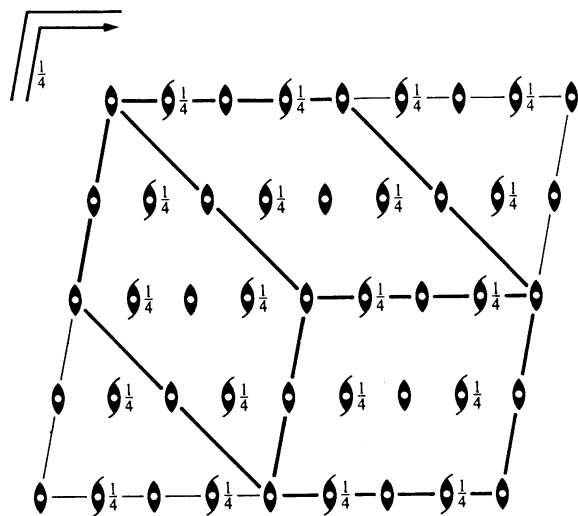
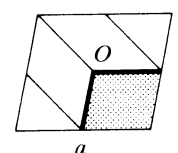
Minimal non-isomorphic supergroups

I	[2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $Fmmm$ (69); [2] $Immm$ (71); [2] $Ibam$ (72); [2] $Imma$ (74); [2] $I4/m$ (87); [3] $P\bar{3}1m$ (162); [3] $P\bar{3}m1$ (164); [3] $R\bar{3}m$ (166)
II	[2] $P112/m$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2/m$, 10)

$C2/m$ C_{2h}^3 $2/m$

Monoclinic

No. 12

UNIQUE AXIS c , DIFFERENT CELL CHOICES $A112/m$ UNIQUE AXIS c , CELL CHOICE 1Origin at centre ($2/m$)Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ 8 j 1 (1) x,y,z (2) \bar{x},\bar{y},z (3) \bar{x},\bar{y},\bar{z} (4) x,y,\bar{z} 4 i m $x,y,0$ $\bar{x},\bar{y},0$ 4 h 2 $\frac{1}{2},0,z$ $\frac{1}{2},0,\bar{z}$ 4 g 2 $0,0,z$ $0,0,\bar{z}$ 4 f $\bar{1}$ $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ 4 e $\bar{1}$ $0, \frac{1}{4}, \frac{1}{4}$ $0, \frac{3}{4}, \frac{1}{4}$ 2 d $2/m$ $\frac{1}{2},0,\frac{1}{2}$ 2 c $2/m$ $\frac{1}{2},0,0$ 2 b $2/m$ $0,0,\frac{1}{2}$ 2 a $2/m$ $0,0,0$

Reflection conditions

General:

 $hkl : k+l = 2n$ $h0l : l = 2n$
 $hk0 : k = 2n$ $00l : l = 2n$
 $0kl : k+l = 2n$ $0k0 : k = 2n$

Special: as above, plus

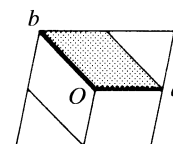
no extra conditions

no extra conditions

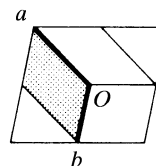
 $hkl : k = 2n$

no extra conditions

no extra conditions

B 1 1 2/mUNIQUE AXIS *c*, CELL CHOICE 2**Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)**Positions**

		Coordinates				Reflection conditions	
Multiplicity, Wyckoff letter, Site symmetry		$(0,0,0)+ (\frac{1}{2},0,\frac{1}{2})+$				General:	
8	<i>j</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) \bar{x},\bar{y},\bar{z}	(4) x,y,\bar{z}	$hkl : h+l=2n$	$h0l : h+l=2n$
						$hk0 : h=2n$	$00l : l=2n$
						$0kl : l=2n$	$h00 : h=2n$
Special: as above, plus							
4	<i>i</i> <i>m</i>	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions	
4	<i>h</i> 2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	4	<i>g</i> 2	$0,0,z$	$0,0,\bar{z}$
						no extra conditions	
4	<i>f</i> $\bar{1}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	4	<i>e</i> $\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$
						$hkl : h=2n$	
2	<i>d</i> $2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		2	<i>c</i> $2/m$	$\frac{1}{2},\frac{1}{2},0$	
						no extra conditions	
2	<i>b</i> $2/m$	$0,0,\frac{1}{2}$		2	<i>a</i> $2/m$	$0,0,0$	
						no extra conditions	

I 1 1 2/mUNIQUE AXIS *c*, CELL CHOICE 3**Origin** at centre ($2/m$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)**Positions**

		Coordinates				Reflection conditions	
Multiplicity, Wyckoff letter, Site symmetry		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:	
8	<i>j</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) \bar{x},\bar{y},\bar{z}	(4) x,y,\bar{z}	$hkl : h+k+l=2n$	$00l : l=2n$
						$hk0 : h+k=2n$	$h00 : h=2n$
						$0kl : k+l=2n$	$0k0 : k=2n$
						$h0l : h+l=2n$	
Special: as above, plus							
4	<i>i</i> <i>m</i>	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions	
4	<i>h</i> 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	4	<i>g</i> 2	$0,0,z$	$0,0,\bar{z}$
						no extra conditions	
4	<i>f</i> $\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	4	<i>e</i> $\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$
						$hkl : l=2n$	
2	<i>d</i> $2/m$	$0,\frac{1}{2},\frac{1}{2}$		2	<i>c</i> $2/m$	$0,\frac{1}{2},0$	
						no extra conditions	
2	<i>b</i> $2/m$	$0,0,\frac{1}{2}$		2	<i>a</i> $2/m$	$0,0,0$	
						no extra conditions	

$P2/c$

C_{2h}^4

$2/m$

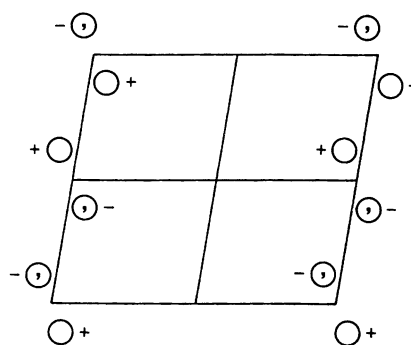
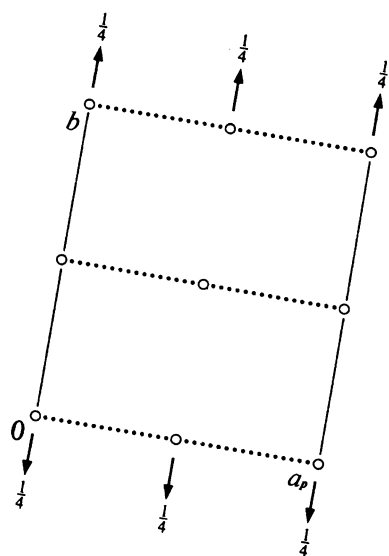
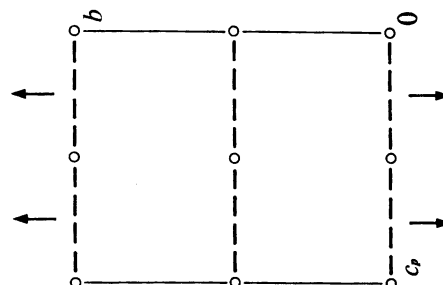
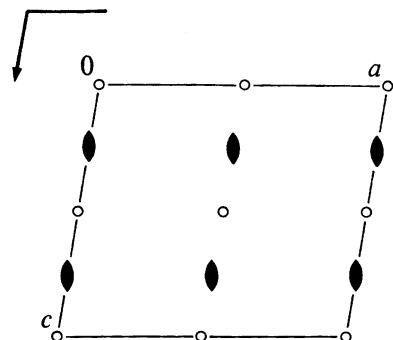
Monoclinic

No. 13

$P12/c1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- (1) 1 (2) $2 \ 0, y, \frac{1}{4}$ (3) $\bar{1} \ 0, 0, 0$ (4) $c \ x, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
4	<i>g</i> 1	(1) x, y, z	(2) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y}, z + \frac{1}{2}$	General: $h0l : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
2	<i>f</i> 2	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$			no extra conditions
2	<i>e</i> 2	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$			no extra conditions
2	<i>d</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : l = 2n$
2	<i>c</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	<i>b</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	<i>a</i> $\bar{1}$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at 0, 0, z

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at x, 0, 0

Along [010] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at 0, y, 0

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc , 7) 1; 4
[2] $P121$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P12_1/c1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_1/c$, 14); [2] $C12/c1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $P12/c1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $P12/c1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$) ($P2/c$, 13)

Minimal non-isomorphic supergroups

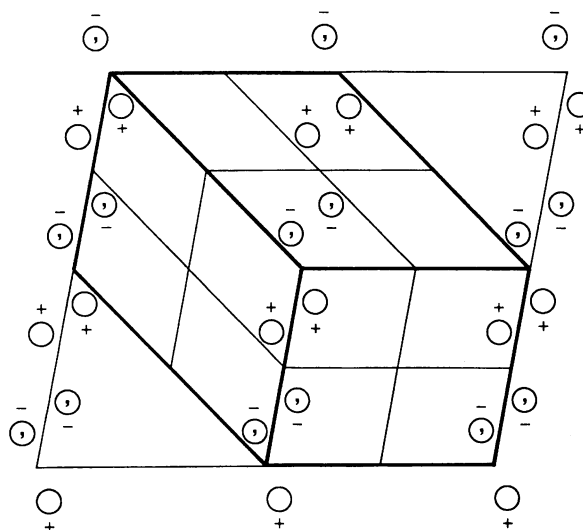
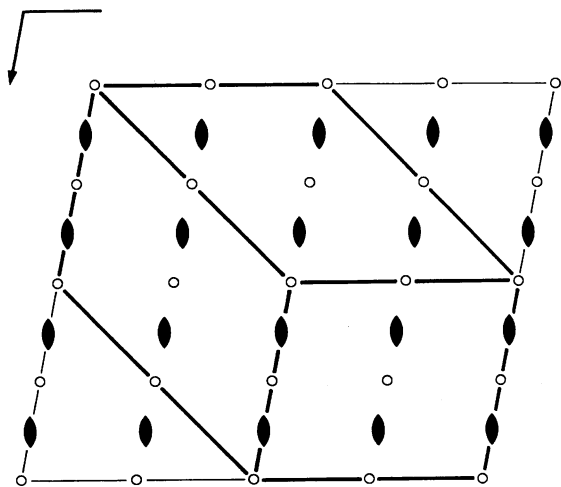
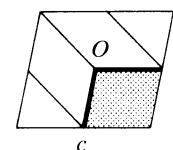
I [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12/m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2/m$, 10)

$P2/c$ C_{2h}^4 $2/m$

Monoclinic

No. 13

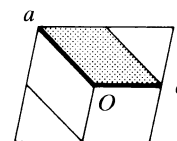
UNIQUE AXIS b , DIFFERENT CELL CHOICES $P12/c1$ UNIQUE AXIS b , CELL CHOICE 1Origin at $\bar{1}$ on glide plane c Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{2}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 g 1	(1) x, y, z (2) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y}, z + \frac{1}{2}$	General: $h0l : l = 2n$ $00l : l = 2n$
2 f 2	$\frac{1}{2}, y, \frac{1}{4}$ $\frac{1}{2}, \bar{y}, \frac{3}{4}$	Special: as above, plus no extra conditions
2 e 2	$0, y, \frac{1}{4}$ $0, \bar{y}, \frac{3}{4}$	no extra conditions
2 d $\bar{1}$	$\frac{1}{2}, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : l = 2n$
2 b $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n$
	2 c $\bar{1}$ $0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$	
	2 a $\bar{1}$ $0, 0, 0$ $0, 0, \frac{1}{2}$	

P12/n1

UNIQUE AXIS b , CELL CHOICE 2**Origin** at $\bar{1}$ on glide plane n **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
4 g 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$
2 f 2	$\frac{3}{4}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \frac{3}{4}$		
2 e 2	$\frac{3}{4}, y, \frac{3}{4}$	$\frac{1}{4}, \bar{y}, \frac{1}{4}$		
2 d $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	2 c $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
2 b $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	2 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$

Reflection conditions

General:

$h0l : h + l = 2n$

$h00 : h = 2n$

$00l : l = 2n$

Special: as above, plus

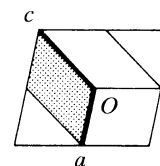
no extra conditions

no extra conditions

$hkl : h + l = 2n$

$hkl : h + l = 2n$

P12/a1

UNIQUE AXIS b , CELL CHOICE 3**Origin** at $\bar{1}$ on glide plane a **Asymmetric unit** $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
4 g 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, y, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, z$
2 f 2	$\frac{3}{4}, y, \frac{1}{2}$	$\frac{1}{4}, \bar{y}, \frac{1}{2}$		
2 e 2	$\frac{1}{4}, y, 0$	$\frac{3}{4}, \bar{y}, 0$		
2 d $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, 0, \frac{1}{2}$	2 c $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
2 b $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	2 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, 0, 0$

Reflection conditions

General:

$h0l : h = 2n$

$h00 : h = 2n$

Special: as above, plus

no extra conditions

no extra conditions

$hkl : h = 2n$

$hkl : h = 2n$

$P2/c$

C_{2h}^4

$2/m$

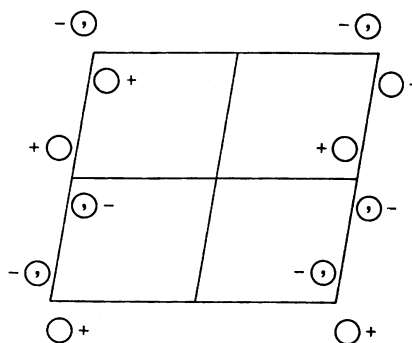
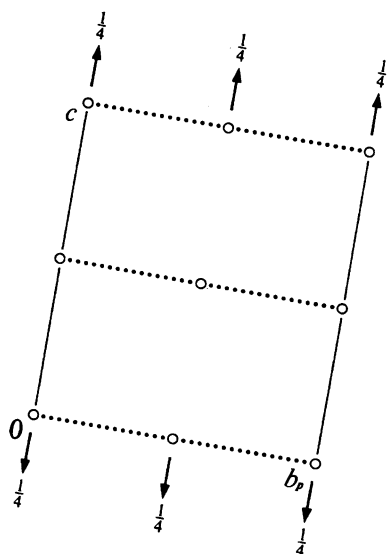
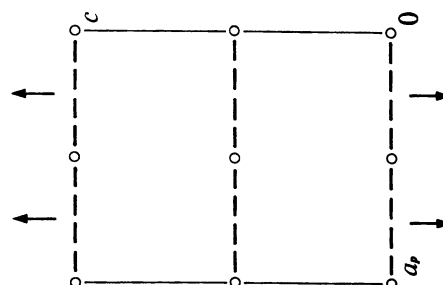
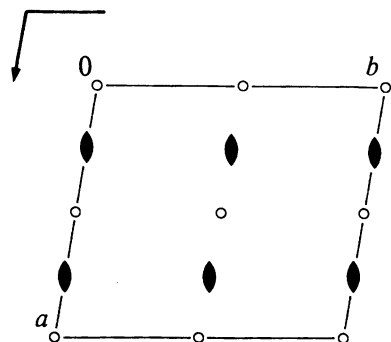
Monoclinic

No. 13

$P112/a$

Patterson symmetry $P112/m$

UNIQUE AXIS c , CELL CHOICE 1



Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2 \frac{1}{4}, 0, z$ (3) $\bar{1} 0, 0, 0$ (4) $a \ x, y, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
4	<i>g</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z}$	General: $hk0 : h = 2n$ $h00 : h = 2n$ Special: as above, plus no extra conditions
2	<i>f</i> 2	$\frac{1}{4}, \frac{1}{2}, z$	$\frac{3}{4}, \frac{1}{2}, \bar{z}$			no extra conditions
2	<i>e</i> 2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z}$			no extra conditions
2	<i>d</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h = 2n$
2	<i>c</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h = 2n$
2	<i>b</i> $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h = 2n$
2	<i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$			$hkl : h = 2n$

Symmetry of special projections

Along [001] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [010] $p2gm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P11a$ (Pc , 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P112_1/a$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1/c$, 14); [2] $A112/a$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $P112/a$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $P112/a$ ($\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13)

Minimal non-isomorphic supergroups

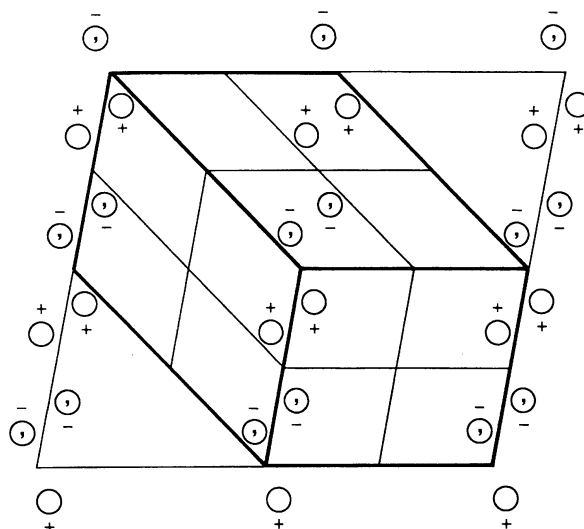
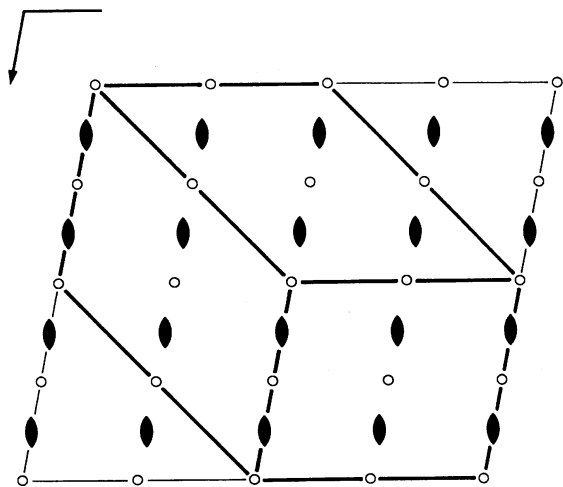
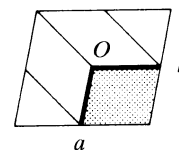
I [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

II [2] $A112/a$ ($C2/c$, 15); [2] $B112/m$ ($C2/m$, 12); [2] $I112/a$ ($C2/c$, 15); [2] $P112/m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($P2/m$, 10)

$P2/c$ C_{2h}^4 $2/m$

Monoclinic

No. 13

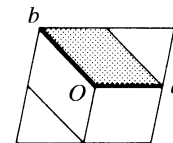
UNIQUE AXIS c , DIFFERENT CELL CHOICES $P112/a$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ on glide plane a Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 g 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x + \frac{1}{2}, y, \bar{z}$	General: $hk0 : h = 2n$ $h00 : h = 2n$
2 f 2	$\frac{1}{4}, \frac{1}{2}, z$ $\frac{3}{4}, \frac{1}{2}, \bar{z}$	Special: as above, plus no extra conditions
2 e 2	$\frac{1}{4}, 0, z$ $\frac{3}{4}, 0, \bar{z}$	no extra conditions
2 d $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h = 2n$
2 b $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h = 2n$
	2 c $\bar{1}$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	
	2 a $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, 0$	

P112/n

UNIQUE AXIS c , CELL CHOICE 2Origin at $\bar{1}$ on glide plane n Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq 1$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 g 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$
2 f 2	$\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$
2 e 2	$\frac{3}{4}, \frac{3}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$
2 d $\bar{1}$	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$
2 b $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$
2 c $\bar{1}$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
2 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$

Reflection conditions

General:

$hk0 : h + k = 2n$

$h00 : h = 2n$

$0k0 : k = 2n$

Special: as above, plus

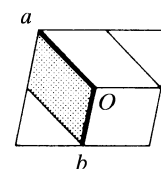
no extra conditions

no extra conditions

$hkl : h + k = 2n$

$hkl : h + k = 2n$

P112/b

UNIQUE AXIS c , CELL CHOICE 3Origin at $\bar{1}$ on glide plane b Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 g 1	(1) x, y, z (2) $\bar{x}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, y + \frac{1}{2}, \bar{z}$
2 f 2	$\frac{1}{2}, \frac{3}{4}, z$ $\frac{1}{2}, \frac{1}{4}, \bar{z}$
2 e 2	$0, \frac{1}{4}, z$ $0, \frac{3}{4}, \bar{z}$
2 d $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$
2 b $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$
2 c $\bar{1}$	$0, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$
2 a $\bar{1}$	$0, 0, 0$ $0, \frac{1}{2}, 0$

Reflection conditions

General:

$hk0 : k = 2n$

$0k0 : k = 2n$

Special: as above, plus

no extra conditions

no extra conditions

$hkl : k = 2n$

$hkl : k = 2n$

$P2_1/c$

C_{2h}^5

$2/m$

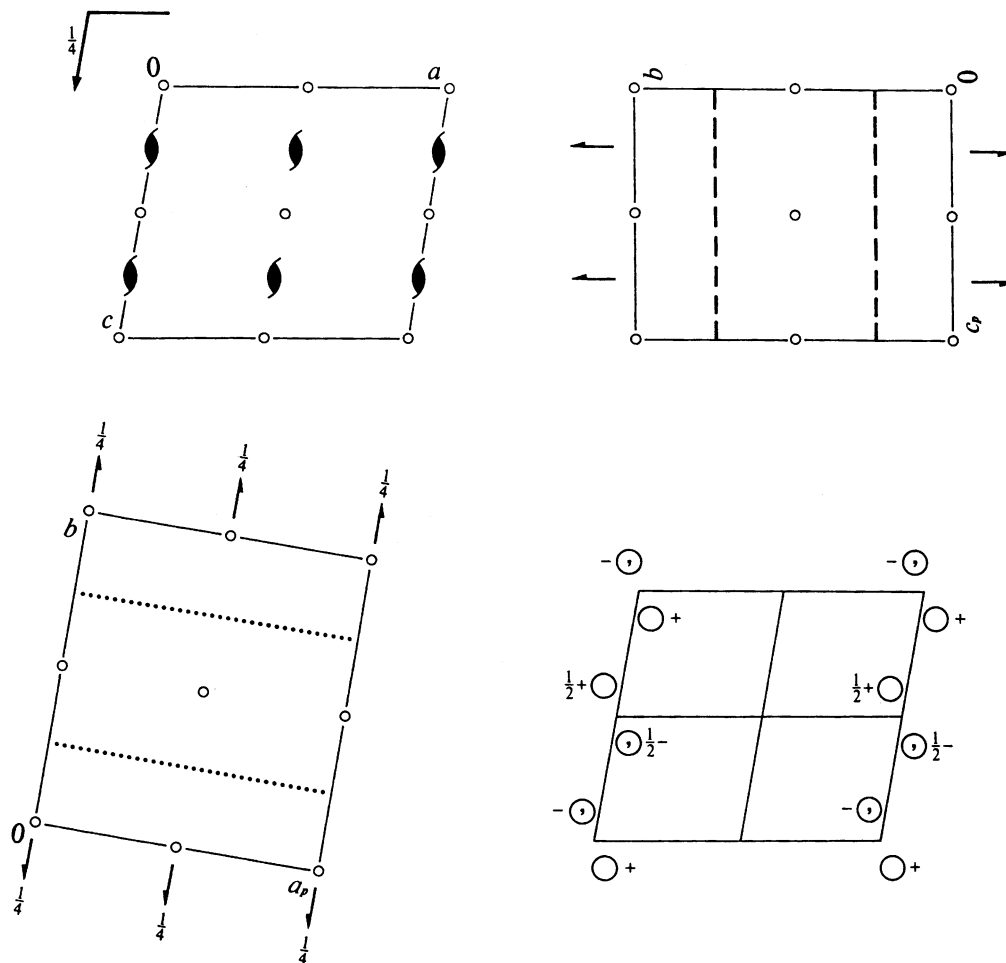
Monoclinic

No. 14

$P12_1/c1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ (3) $\bar{1}$ $0, 0, 0$ (4) c $x, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>e</i> 1	(1) x, y, z	(2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	General: $h0l : l = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : k + l = 2n$ $hkl : k + l = 2n$ $hkl : k + l = 2n$ $hkl : k + l = 2n$
2 <i>d</i> $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : k + l = 2n$
2 <i>c</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$			$hkl : k + l = 2n$
2 <i>b</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : k + l = 2n$
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : k + l = 2n$

Symmetry of special projections

Along $[001]$ $p2gm$

$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along $[100]$ $p2gg$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$

Origin at $x, 0, 0$

Along $[010]$ $p2$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I $[2] P1c1 (Pc, 7)$ 1; 4
 $[2] P12_11 (P2_1, 4)$ 1; 2
 $[2] P\bar{1} (2)$ 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2] P12_1/c1 (\mathbf{a}' = 2\mathbf{a} \text{ or } \mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}) (P2_1/c, 14)$; $[3] P12_1/c1 (\mathbf{b}' = 3\mathbf{b}) (P2_1/c, 14)$

Minimal non-isomorphic supergroups

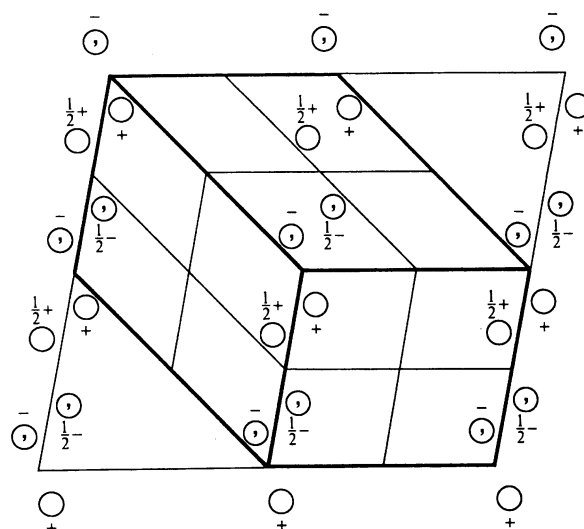
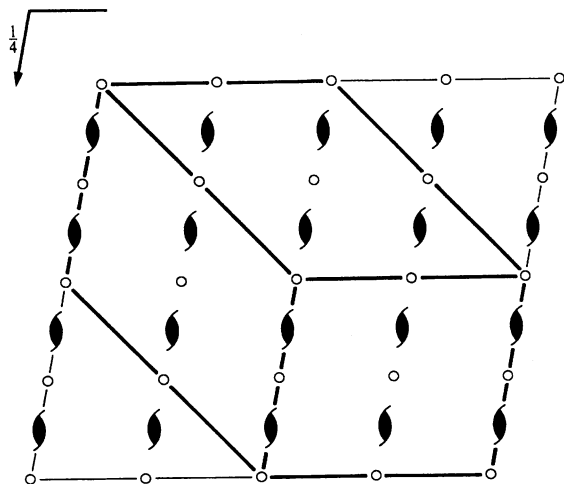
I $[2] Pnna (52)$; $[2] Pmna (53)$; $[2] Pcca (54)$; $[2] Pbam (55)$; $[2] Pccn (56)$; $[2] Pbcm (57)$; $[2] Pnnm (58)$; $[2] Pbcn (60)$;
 $[2] Pbca (61)$; $[2] Pnma (62)$; $[2] Cmce (64)$

II $[2] A12/m1 (C2/m, 12)$; $[2] C12/c1 (C2/c, 15)$; $[2] I12/c1 (C2/c, 15)$; $[2] P12_1/m1 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2_1/m, 11)$;
 $[2] P12/c1 (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (P2/c, 13)$

$P2_1/c$ C_{2h}^5 $2/m$

Monoclinic

No. 14

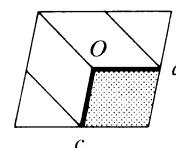
UNIQUE AXIS b , DIFFERENT CELL CHOICES $P12_1/c1$ UNIQUE AXIS b , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 e 1	(1) x, y, z (2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$
2 d $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$
2 c $\bar{1}$	$0, 0, \frac{1}{2}$ $0, \frac{1}{2}, 0$
2 b $\bar{1}$	$\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
2 a $\bar{1}$	$0, 0, 0$ $0, \frac{1}{2}, \frac{1}{2}$



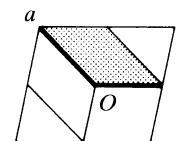
Reflection conditions

General:

 $h0l : l = 2n$
 $0k0 : k = 2n$
 $00l : l = 2n$

Special: as above, plus

 $hkl : k + l = 2n$ $hkl : k + l = 2n$ $hkl : k + l = 2n$ $hkl : k + l = 2n$

$P12_1/n1$ UNIQUE AXIS b , CELL CHOICE 2Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4	e	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$
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Reflection conditions

General:

$h0l : h + l = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

$00l : l = 2n$

Special: as above, plus

2	d	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
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$hkl : h + k + l = 2n$

2	c	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$
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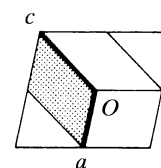
$hkl : h + k + l = 2n$

2	b	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
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$hkl : h + k + l = 2n$

2	a	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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$hkl : h + k + l = 2n$

 $P12_1/a1$ UNIQUE AXIS b , CELL CHOICE 3Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4	e	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$
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Reflection conditions

General:

$h0l : h = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

Special: as above, plus

2	d	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	---------------------	---

$hkl : h + k = 2n$

2	c	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$
---	-----	-----------	---------------------	---------------------

$hkl : h + k = 2n$

2	b	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$
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$hkl : h + k = 2n$

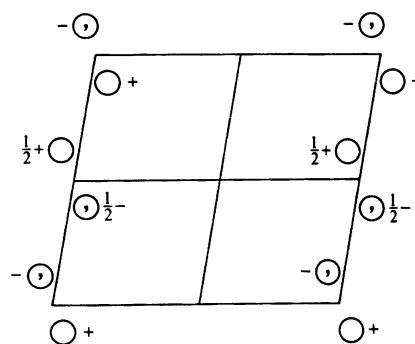
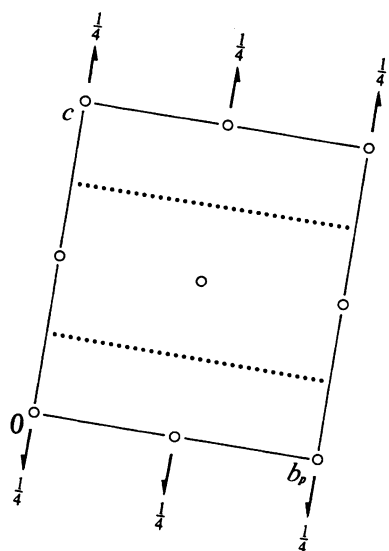
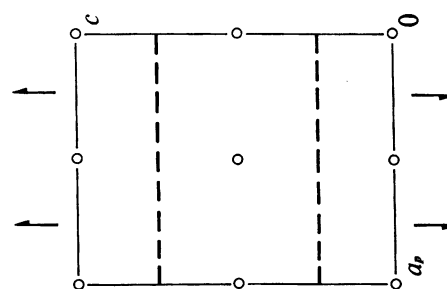
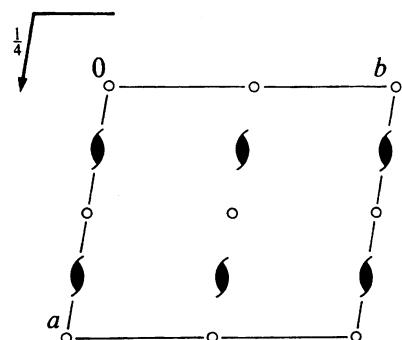
2	a	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$
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$hkl : h + k = 2n$

$P2_1/c$ C_{2h}^5 $2/m$

Monoclinic

No. 14

 $P112_1/a$ Patterson symmetry $P112/m$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- (1) 1 (2) $2(0, 0, \frac{1}{2}) \frac{1}{4}, 0, z$ (3) $\bar{1} 0, 0, 0$ (4) $a \ x, y, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>e</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	General: $hk0 : h = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus $hkl : h + l = 2n$
2 <i>d</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + l = 2n$
2 <i>c</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : h + l = 2n$
2 <i>b</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + l = 2n$
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + l = 2n$

Symmetry of special projections

Along $[001]$ $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $p2gm$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[010]$ $p2gg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I $[2] P11a (Pc, 7)$ 1; 4
 $[2] P112_1 (P2_1, 4)$ 1; 2
 $[2] P\bar{1} (2)$ 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2] P112_1/a (\mathbf{b}' = 2\mathbf{b} \text{ or } \mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = 2\mathbf{b}) (P2_1/c, 14)$; $[3] P112_1/a (\mathbf{c}' = 3\mathbf{c}) (P2_1/c, 14)$

Minimal non-isomorphic supergroups

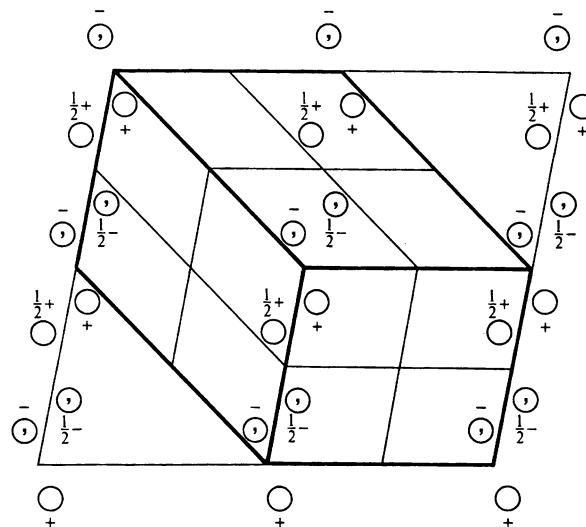
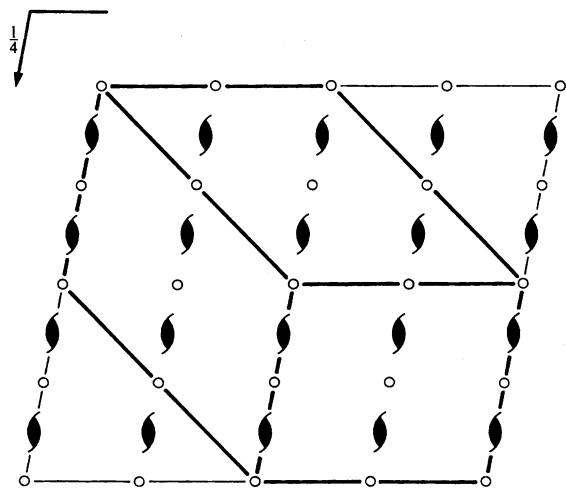
I $[2] Pnna (52)$; $[2] Pmna (53)$; $[2] Pcca (54)$; $[2] Pbam (55)$; $[2] Pccn (56)$; $[2] Pbcm (57)$; $[2] Pnnm (58)$; $[2] Pbcn (60)$;
 $[2] Pbca (61)$; $[2] Pnma (62)$; $[2] Cmce (64)$

II $[2] A112/a (C2/c, 15)$; $[2] B112/m (C2/m, 12)$; $[2] I112/a (C2/c, 15)$; $[2] P112_1/m (\mathbf{a}' = \frac{1}{2}\mathbf{a}) (P2_1/m, 11)$;
 $[2] P112/a (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P2/c, 13)$

$P2_1/c$ C_{2h}^5 $2/m$

Monoclinic

No. 14

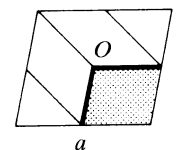
UNIQUE AXIS c , DIFFERENT CELL CHOICES $P112_1/a$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 e $\bar{1}$	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$
2 d $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$
2 c $\bar{1}$	$\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$
2 b $\bar{1}$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
2 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$



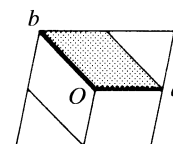
Reflection conditions

General:

 $hk0 : h = 2n$
 $00l : l = 2n$
 $h00 : h = 2n$

Special: as above, plus

 $hkl : h + l = 2n$ $hkl : h + l = 2n$ $hkl : h + l = 2n$ $hkl : h + l = 2n$

$P112_1/n$ UNIQUE AXIS c , CELL CHOICE 2Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4	e	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$
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Reflection conditions

General:

 $hk0 : h + k = 2n$ $00l : l = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$

Special: as above, plus

2	d	$\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$
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 $hkl : h + k + l = 2n$

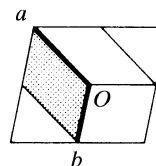
2	c	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
---	-----	-----------	-------------------------------	---------------------

 $hkl : h + k + l = 2n$

2	b	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	---------------------	-------------------------------

 $hkl : h + k + l = 2n$

2	a	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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 $hkl : h + k + l = 2n$ $P112_1/b$ UNIQUE AXIS c , CELL CHOICE 3Origin at $\bar{1}$ Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4	e	1	(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$
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Reflection conditions

General:

 $hk0 : k = 2n$ $00l : l = 2n$ $0k0 : k = 2n$

Special: as above, plus

2	d	$\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	---------------------	---

 $hkl : k + l = 2n$

2	c	$\bar{1}$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
---	-----	-----------	---------------------	---------------------

 $hkl : k + l = 2n$

2	b	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$
---	-----	-----------	-------------------------------	-------------------------------

 $hkl : k + l = 2n$

2	a	$\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	-----------	-------------------------------

 $hkl : k + l = 2n$

$C2/c$

C_{2h}^6

$2/m$

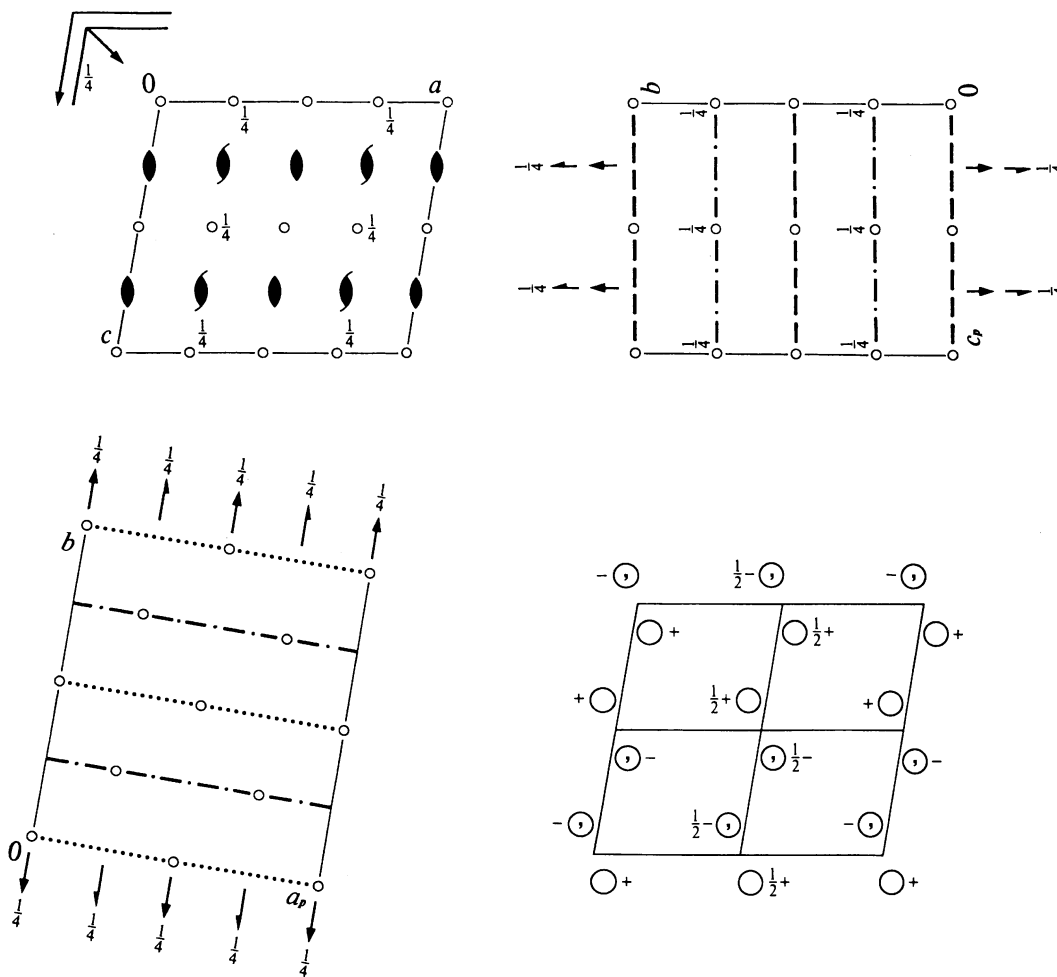
Monoclinic

No. 15

$C12/c1$

Patterson symmetry $C12/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2 \quad 0, y, \frac{1}{4}$ (3) $\bar{1} \quad 0, 0, 0$ (4) $c \quad x, 0, z$

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ (2) $2(0, \frac{1}{2}, 0) \quad \frac{1}{4}, y, \frac{1}{4}$ (3) $\bar{1} \quad \frac{1}{4}, \frac{1}{4}, 0$ (4) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8 <i>f</i> 1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) \bar{x},\bar{y},\bar{z}	(4) $x,\bar{y},z+\frac{1}{2}$	$hkl : h+k=2n$ $h0l : h,l=2n$ $0kl : k=2n$ $hk0 : h+k=2n$ $0k0 : k=2n$ $h00 : h=2n$ $00l : l=2n$
					Special: as above, plus
4 <i>e</i> 2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			$hkl : k+l=2n$
4 <i>c</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : k+l=2n$
4 <i>b</i> $\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : l=2n$
4 <i>a</i> $\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			$hkl : l=2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
 Origin at x,0,0

Along [010] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C1c1$ (Cc , 9)	(1; 4)+
	[2] $C121$ ($C2$, 5)	(1; 2)+
	[2] $C\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P12_1/n1$ ($P2_1/c$, 14)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12_1/c1$ ($P2_1/c$, 14)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12/c1$ ($P2/c$, 13)	1; 2; 3; 4
	[2] $P12/n1$ ($P2/c$, 13)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $C12/c1$ ($\mathbf{b}' = 3\mathbf{b}$) ($C2/c$, 15); [3] $C12/c1$ ($\mathbf{c}' = 3\mathbf{c}$) ($C2/c$, 15);
 [3] $C12/c1$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = -\mathbf{a} + \mathbf{c}$ or $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$) ($C2/c$, 15)

Minimal non-isomorphic supergroups

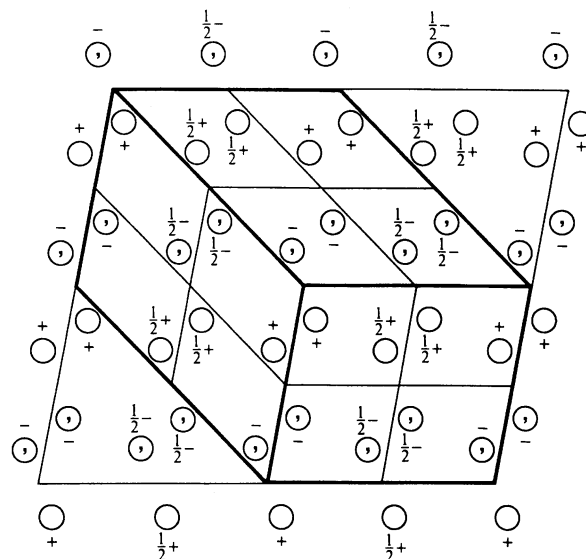
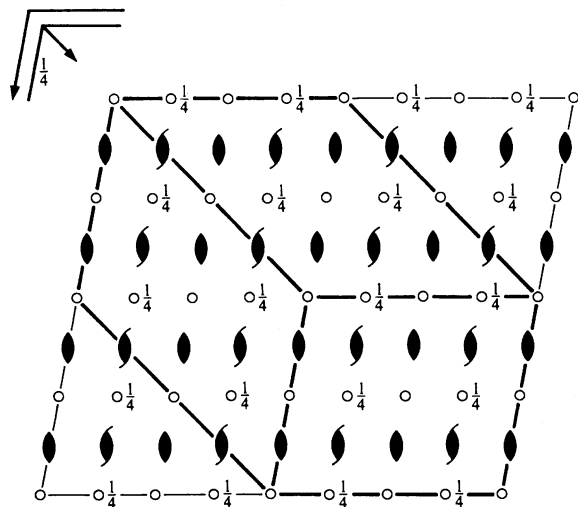
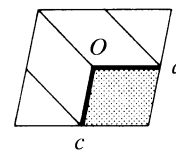
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74);
 [2] $I4_1/a$ (88); [3] $P\bar{3}1c$ (163); [3] $P\bar{3}c1$ (165); [3] $R\bar{3}c$ (167)

II [2] $F12/m1$ ($C2/m$, 12); [2] $C12/m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($C2/m$, 12); [2] $P12/c1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

$C2/c$ C_{2h}^6 $2/m$

Monoclinic

No. 15

UNIQUE AXIS b , DIFFERENT CELL CHOICES $C12/c1$ UNIQUE AXIS b , CELL CHOICE 1Origin at $\bar{1}$ on glide plane c Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, 0)$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

 $(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, 0)+$

General:

8 f 1 (1) x,y,z (2) $\bar{x},y,\bar{z}+\frac{1}{2}$ (3) \bar{x},\bar{y},\bar{z} (4) $x,\bar{y},z+\frac{1}{2}$
 $hkl : h+k=2n$ $0k0 : k=2n$
 $h0l : h,l=2n$ $h00 : h=2n$
 $0kl : k=2n$ $00l : l=2n$
 $hk0 : h+k=2n$

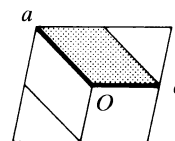
Special: as above, plus

4	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},0$	4	c	$\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	4	a	$\bar{1}$ $0,0,0$ $0,0,\frac{1}{2}$

no extra conditions

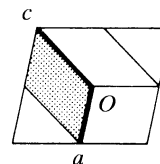
 $hkl : k+l=2n$ $hkl : l=2n$

A12/n1

UNIQUE AXIS b , CELL CHOICE 2**Origin** at $\bar{1}$ on glide plane n **Asymmetric unit** $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$				General:
8 f 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	$hkl : k + l = 2n$ $0k0 : k = 2n$ $h0l : h, l = 2n$ $h00 : h = 2n$ $0kl : k + l = 2n$ $00l : l = 2n$ $hk0 : k = 2n$
4 e 2	$\frac{3}{4}, y, \frac{3}{4}$	$\frac{1}{4}, \bar{y}, \frac{1}{4}$			Special: as above, plus no extra conditions
4 d $\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$0, \frac{1}{4}, \frac{3}{4}$	4 c $\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$hkl : h = 2n$
4 b $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	4 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k = 2n$

I12/a1

UNIQUE AXIS b , CELL CHOICE 3**Origin** at $\bar{1}$ on glide plane a **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
8 f 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, y, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, z$	$hkl : h + k + l = 2n$ $0k0 : k = 2n$ $h0l : h, l = 2n$ $h00 : h = 2n$ $0kl : k + l = 2n$ $00l : l = 2n$ $hk0 : h + k = 2n$
4 e 2	$\frac{1}{4}, y, 0$	$\frac{3}{4}, \bar{y}, 0$			Special: as above, plus no extra conditions
4 d $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	4 c $\bar{1}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : l = 2n$
4 b $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	4 a $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, 0, 0$	$hkl : h = 2n$

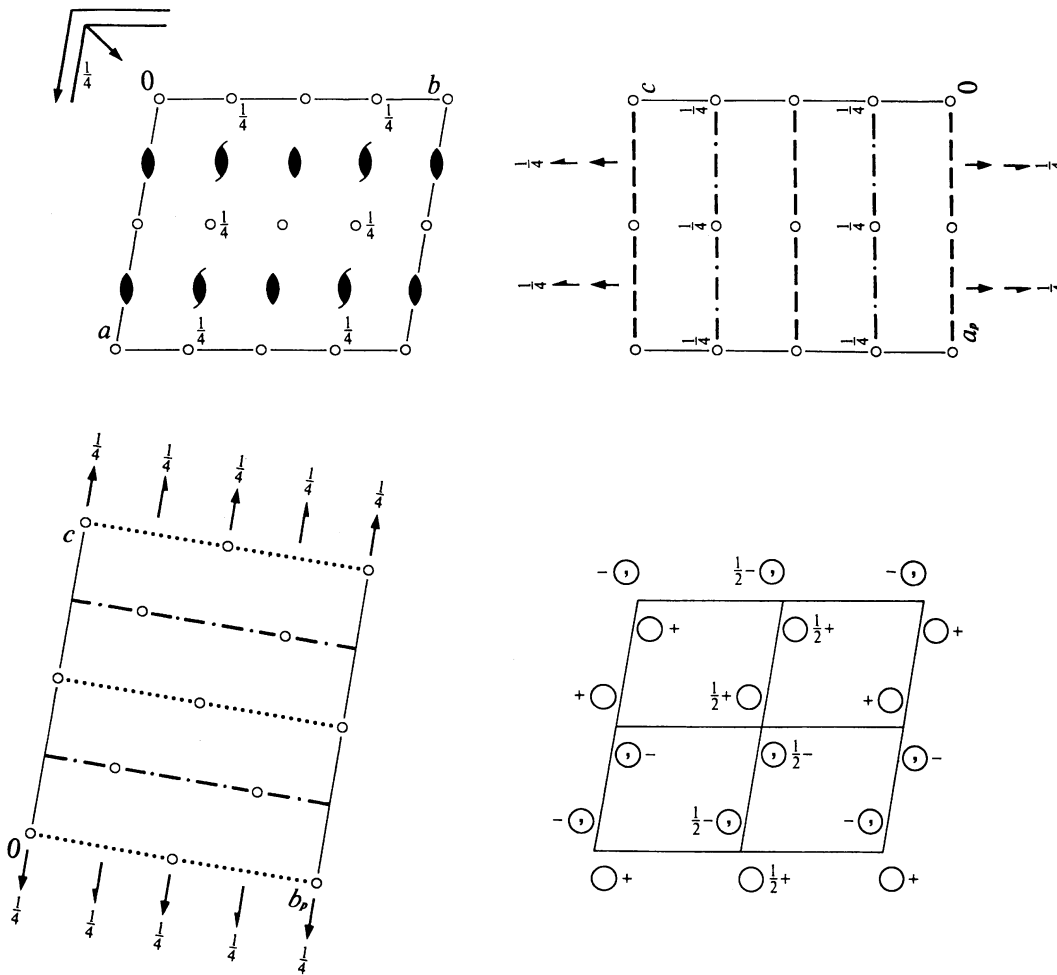
$C2/c$ C_{2h}^6 $2/m$

Monoclinic

No. 15

A112/a

Patterson symmetry A112/m

UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ on glide plane a Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-------|---------------------------|-----------------------|-------------------|
| (1) 1 | (2) $2 \frac{1}{4}, 0, z$ | (3) $\bar{1} 0, 0, 0$ | (4) $a \ x, y, 0$ |
|-------|---------------------------|-----------------------|-------------------|

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--------------------------------------|--|---|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \ \frac{1}{4}, \frac{1}{4}, z$ | (3) $\bar{1} 0, \frac{1}{4}, \frac{1}{4}$ | (4) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, \frac{1}{4}$ |
|--------------------------------------|--|---|--|

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+			General:
8 <i>f</i> 1	(1) x,y,z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, y, \bar{z}$	$hkl : k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $h0l : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$
					Special: as above, plus
4 <i>e</i> 2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z}$			no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$			$hkl : h + k = 2n$
4 <i>c</i> $\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$			$hkl : h + k = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$			$hkl : h = 2n$

Symmetry of special projections

Along [001] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0, 0, z

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
 Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $A11a$ (Cc , 9)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
	[2] $A\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P112_1/n$ ($P2_1/c$, 14)	1; 3; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 4; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $P112/a$ ($P2/c$, 13)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $A112/a$ ($\mathbf{c}' = 3\mathbf{c}$) ($C2/c$, 15); [3] $A112/a$ ($\mathbf{a}' = 3\mathbf{a}$) ($C2/c$, 15);
 [3] $A112/a$ ($\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = 3\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = 3\mathbf{b}$) ($C2/c$, 15)

Minimal non-isomorphic supergroups

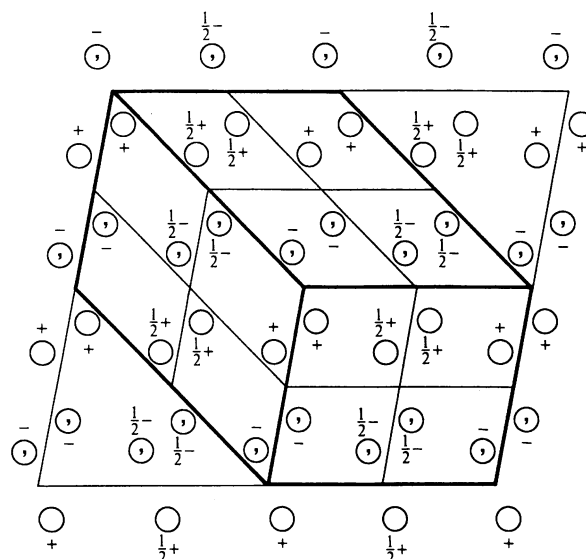
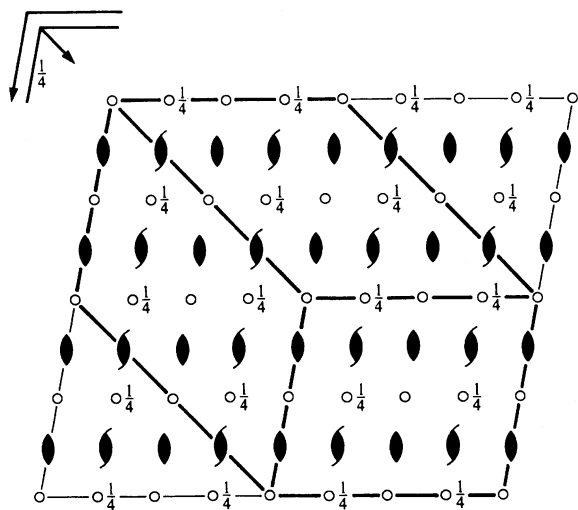
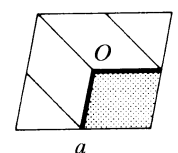
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74);
 [2] $I4_1/a$ (88); [3] $P\bar{3}1c$ (163); [3] $P\bar{3}c1$ (165); [3] $R\bar{3}c$ (167)

II [2] $F112/m$ ($C2/m$, 12); [2] $A112/m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($C2/m$, 12); [2] $P112/a$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2/c$, 13)

$C2/c$ C_{2h}^6 $2/m$

Monoclinic

No. 15

UNIQUE AXIS c , DIFFERENT CELL CHOICES $A112/a$ UNIQUE AXIS c , CELL CHOICE 1Origin at $\bar{1}$ on glide plane a Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$ Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

 $(0,0,0)+ (0, \frac{1}{2}, \frac{1}{2})+$

General:

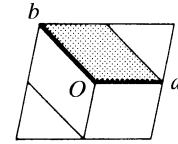
8 f 1 (1) x,y,z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x + \frac{1}{2}, y, \bar{z}$
 $hkl : k+l = 2n$ $00l : l = 2n$
 $hk0 : h, k = 2n$ $h00 : h = 2n$
 $0kl : k+l = 2n$ $0k0 : k = 2n$
 $h0l : l = 2n$

Special: as above, plus

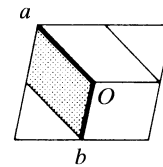
4	e	2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z}$			
4	d	$\bar{1}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	4	c	$\bar{1}$ $0, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$
4	b	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	4	a	$\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, 0$

no extra conditions

 $hkl : h+k = 2n$ $hkl : h = 2n$

B112/nUNIQUE AXIS *c*, CELL CHOICE 2**Origin** at $\bar{1}$ on glide plane *n***Asymmetric unit** $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},0,\frac{1}{2})+$				General:
8 <i>f</i> 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) \bar{x},\bar{y},\bar{z}	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	$hkl : h+l=2n$ $00l : l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0kl : l=2n$ $0k0 : k=2n$ $h0l : h+l=2n$
4 <i>e</i> 2	$\frac{3}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$			Special: as above, plus no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$	4 <i>c</i> $\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$ $\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$hkl : k=2n$
4 <i>b</i> $\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	4 <i>a</i> $\bar{1}$	$0,0,0$ $\frac{1}{2},\frac{1}{2},0$	$hkl : h+k=2n$

I112/bUNIQUE AXIS *c*, CELL CHOICE 3**Origin** at $\bar{1}$ on glide plane *b***Asymmetric unit** $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{2}$ **Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8 <i>f</i> 1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z$	(3) \bar{x},\bar{y},\bar{z}	(4) $x,y+\frac{1}{2},\bar{z}$	$hkl : h+k+l=2n$ $00l : l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0kl : k+l=2n$ $0k0 : k=2n$ $h0l : h+l=2n$
4 <i>e</i> 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			Special: as above, plus no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	4 <i>c</i> $\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$hkl : h=2n$
4 <i>b</i> $\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	4 <i>a</i> $\bar{1}$	$0,0,0$ $0,\frac{1}{2},0$	$hkl : k=2n$

P222

D_2^1

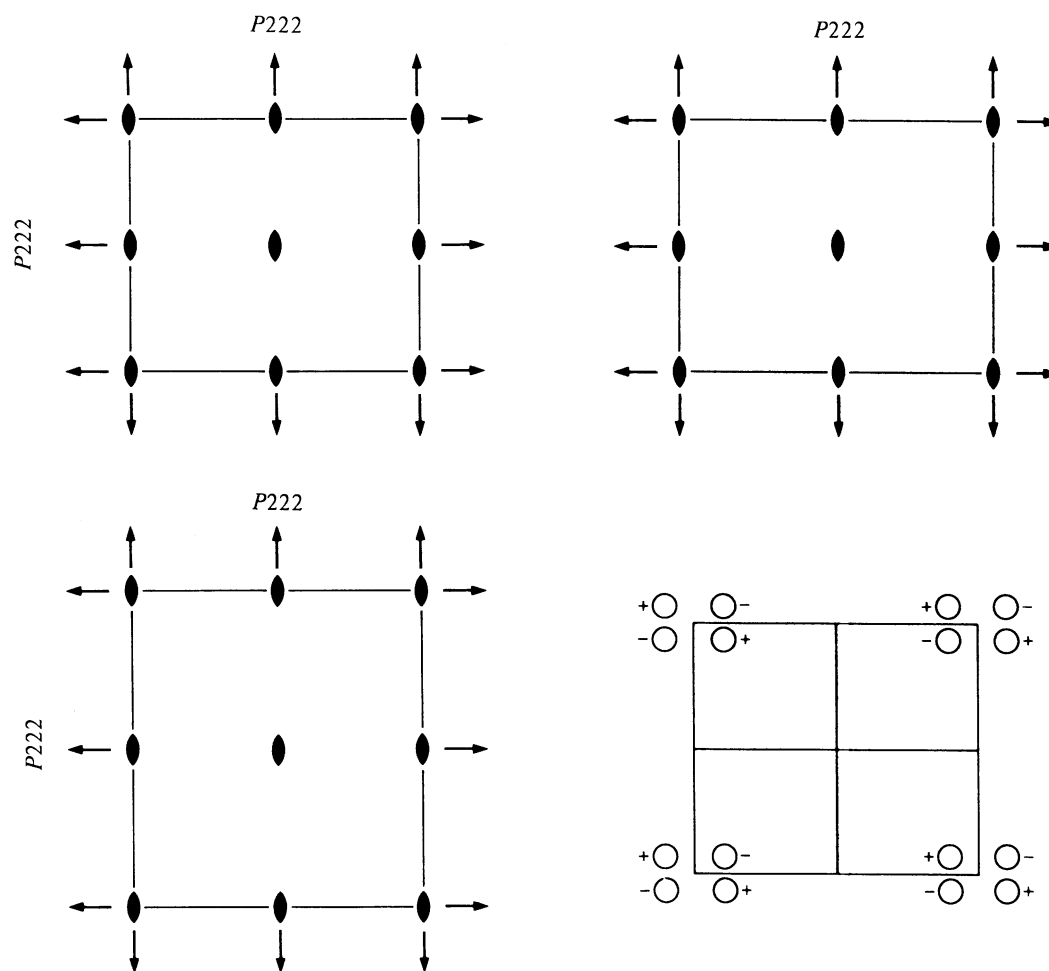
222

Orthorhombic

No. 16

P222

Patterson symmetry *Pmmm*



Origin at 222

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) 2 0,0,z (3) 2 0,y,0 (4) 2 x,0,0

Maximal non-isomorphic subgroups

I [2] *P112* (*P2*, 3) 1; 2
 [2] *P121* (*P2*, 3) 1; 3
 [2] *P211* (*P2*, 3) 1; 4

IIa none

IIb [2] *P2₁22* ($\mathbf{a}' = 2\mathbf{a}$) (*P222₁*, 17); [2] *P2₂22* ($\mathbf{b}' = 2\mathbf{b}$) (*P222₁*, 17); [2] *P222₁* ($\mathbf{c}' = 2\mathbf{c}$) (17);
 [2] *A222* ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (*C222*, 21); [2] *B222* ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) (*C222*, 21); [2] *C222* ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (21);
 [2] *F222* ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (22)

Maximal isomorphic subgroups of lowest index

IIc [2] *P222* ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$) (16)

Minimal non-isomorphic supergroups

I [2] *Pmmm* (47); [2] *Pnnn* (48); [2] *Pccm* (49); [2] *Pban* (50); [2] *P422* (89); [2] *P4₂22* (93); [2] *P4₂c* (112); [2] *P4₂m* (111);
 [3] *P23* (195)
II [2] *A222* (*C222*, 21); [2] *B222* (*C222*, 21); [2] *C222* (21); [2] *I222* (23)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	General: no conditions Special: no extra conditions
4 <i>u</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	
2 <i>t</i> ..2	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			
2 <i>s</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$			
2 <i>r</i> ..2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$			
2 <i>q</i> ..2	$0, 0, z$	$0, 0, \bar{z}$			
2 <i>p</i> .2.	$\frac{1}{2}, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$			
2 <i>o</i> .2.	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$			
2 <i>n</i> .2.	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$			
2 <i>m</i> .2.	$0, y, 0$	$0, \bar{y}, 0$			
2 <i>l</i> 2..	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$			
2 <i>k</i> 2..	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$			
2 <i>j</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$			
2 <i>i</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$			
1 <i>h</i> 222	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				
1 <i>g</i> 222	$0, \frac{1}{2}, \frac{1}{2}$				
1 <i>f</i> 222	$\frac{1}{2}, 0, \frac{1}{2}$				
1 <i>e</i> 222	$\frac{1}{2}, \frac{1}{2}, 0$				
1 <i>d</i> 222	$0, 0, \frac{1}{2}$				
1 <i>c</i> 222	$0, \frac{1}{2}, 0$				
1 <i>b</i> 222	$\frac{1}{2}, 0, 0$				
1 <i>a</i> 222	$0, 0, 0$				

Symmetry of special projections

Along [001] $p2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

(Continued on preceding page)

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [010] $p2mm$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $0, y, 0$

$P222_1$

D_2^2

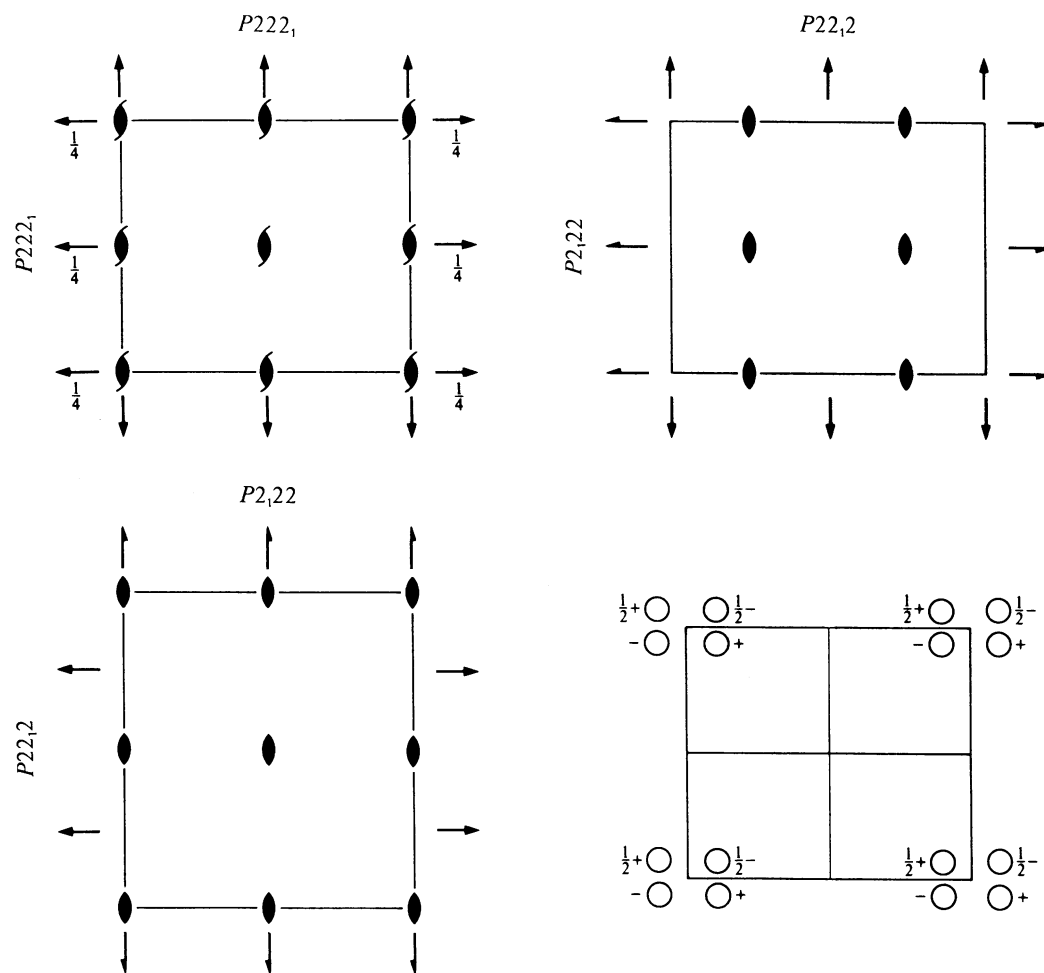
222

Orthorhombic

No. 17

$P222_1$

Patterson symmetry $Pmmm$



Origin at 212_1

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $2(0,y,\frac{1}{4})$ (4) $2(x,0,0)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>e</i> 1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(4) x, \bar{y}, \bar{z}	General: $00l : l = 2n$ Special: as above, plus $h0l : l = 2n$ $h0l : l = 2n$ $0kl : l = 2n$ $0kl : l = 2n$
2 <i>d</i> .2.	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$			
2 <i>c</i> .2.	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$			
2 <i>b</i> 2..	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$			
2 <i>a</i> 2..	$x, 0, 0$	$\bar{x}, 0, \frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [010] $p2mg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0, y, \frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P112_1$ ($P2_1, 4$) 1; 2
[2] $P121$ ($P2, 3$) 1; 3
[2] $P211$ ($P2, 3$) 1; 4

IIa none

IIb [2] $P2_122_1$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2_12_12, 18$); [2] $P22_12_1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_12_12, 18$); [2] $C222_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (20)

Maximal isomorphic subgroups of lowest index

IIc [2] $P222_1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (17); [3] $P222_1$ ($\mathbf{c}' = 3\mathbf{c}$) (17)

Minimal non-isomorphic supergroups

I [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $P4_122$ (91); [2] $P4_322$ (95)

II [2] $C222_1$ (20); [2] $A222$ ($C222, 21$); [2] $B222$ ($C222, 21$); [2] $I2_12_12_1$ (24); [2] $P222$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (16)

$P2_12_12$

D_2^3

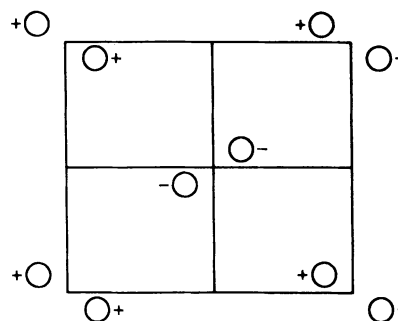
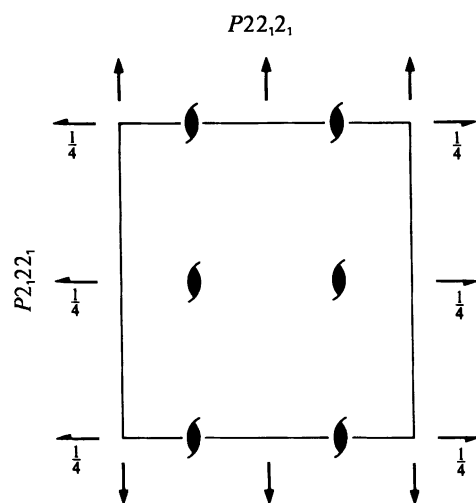
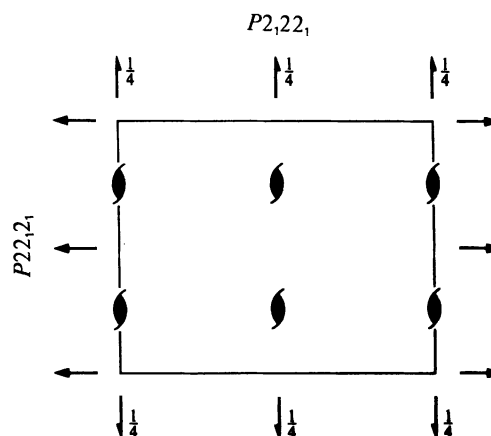
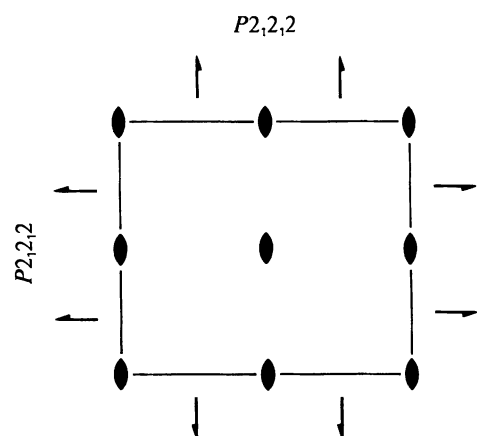
222

Orthorhombic

No. 18

$P2_12_12$

Patterson symmetry $Pmmm$



Origin at intersection of 2 with perpendicular plane containing 2_1 axes

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2 \ 0,0,z$ (3) $2(0,\frac{1}{2},0) \ \frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0) \ x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$h00: h = 2n$ $0k0: k = 2n$
2 <i>b</i> ..2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			Special: as above, plus $hk0: h + k = 2n$
2 <i>a</i> ..2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			$hk0: h + k = 2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, 0$

Along [010] $p2gm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $\frac{1}{4}, y, 0$

Maximal non-isomorphic subgroups

I [2] $P12_11$ ($P2_1, 4$) 1; 3
 [2] $P2_111$ ($P2_1, 4$) 1; 4
 [2] $P1112$ ($P2, 3$) 1; 2

IIa none

IIIb [2] $P2_12_12_1$ ($\mathbf{c}' = 2\mathbf{c}$) (19)

Maximal isomorphic subgroups of lowest index

IIIc [2] $P2_12_12$ ($\mathbf{c}' = 2\mathbf{c}$) (18); [3] $P2_12_12$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (18)

Minimal non-isomorphic supergroups

I [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnmm$ (58); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $P4_22$ (90); [2] $P4_22_12$ (94);
 [2] $P\bar{4}2_1m$ (113); [2] $P\bar{4}2_1c$ (114)

II [2] $A2_122$ ($C222_1, 20$); [2] $B2_12_12$ ($C222_1, 20$); [2] $C222$ (21); [2] $I222$ (23); [2] $P22_12$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($P222_1, 17$);
 [2] $P2_122$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P222_1, 17$)

$P2_12_12_1$

D_2^4

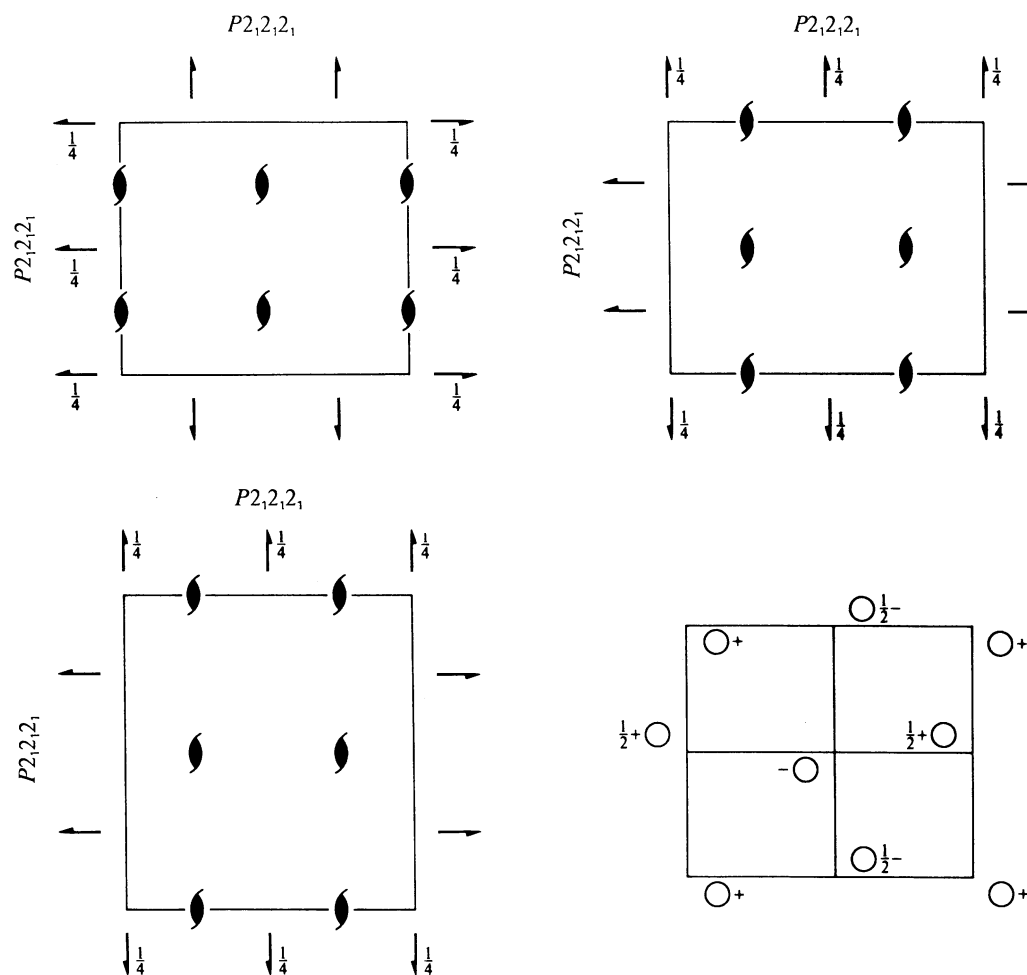
222

Orthorhombic

No. 19

$P2_12_12_1$

Patterson symmetry $Pmmm$



Origin at midpoint of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, 0, \frac{1}{2}) \frac{1}{4}, 0, z$ (3) $2(0, \frac{1}{2}, 0) 0, y, \frac{1}{4}$ (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{4}, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>a</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $\frac{1}{4}, 0, z$

Along [100] $p2gg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, 0$

Along [010] $p2gg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, \frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P112_1 (P2_1, 4)$ 1; 2
 [2] $P12_11 (P2_1, 4)$ 1; 3
 [2] $P2_111 (P2_1, 4)$ 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P2_12_12_1 (\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c})$ (19)

Minimal non-isomorphic supergroups

I [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $P4_12_12$ (92); [2] $P4_32_12$ (96); [3] $P2_13$ (198)

II [2] $A2_122 (C222_1, 20)$; [2] $B22_12 (C222_1, 20)$; [2] $C222_1$ (20); [2] $I2_12_12_1$ (24); [2] $P22_12_1 (\mathbf{a}' = \frac{1}{2}\mathbf{a})$ ($P2_12_12, 18$);
 [2] $P2_122_1 (\mathbf{b}' = \frac{1}{2}\mathbf{b})$ ($P2_12_12, 18$); [2] $P2_12_12 (\mathbf{c}' = \frac{1}{2}\mathbf{c})$ (18)

$C222_1$

D_2^5

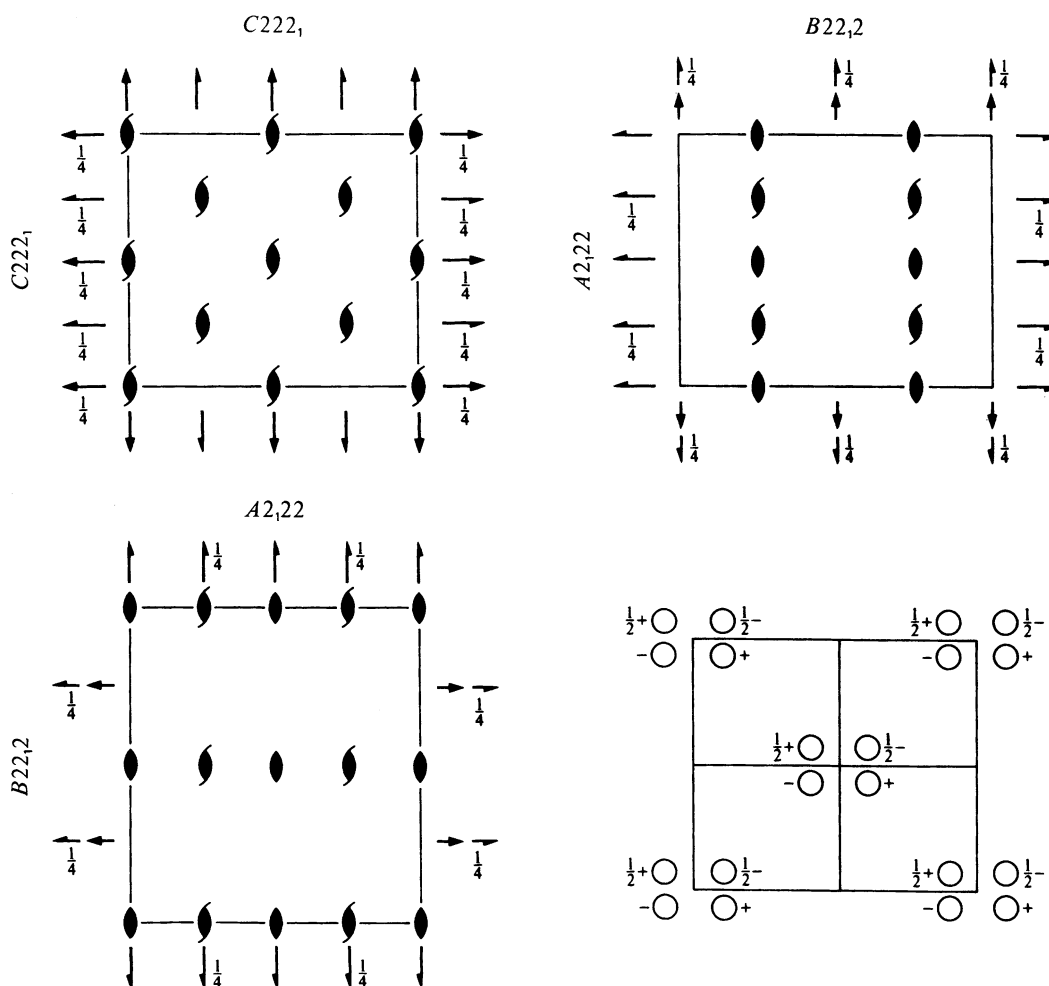
222

Orthorhombic

No. 20

$C222_1$

Patterson symmetry $Cmmm$



Origin at 212_1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1
- (2) $2(0,0,\frac{1}{2})$ $0,0,z$
- (3) $2(0,y,\frac{1}{4})$
- (4) $2(x,0,0)$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$
- (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
- (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$
- (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
8 c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) x,\bar{y},\bar{z}	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
4 b .2.	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			Special: as above, plus $h0l : l=2n$
4 a 2..	$x,0,0$	$\bar{x},0,\frac{1}{2}$			$0kl : l=2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0,0,z

Along [100] $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at x,0,0

Along [010] $p2mg$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at 0,y, $\frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $C121 (C2, 5)$	(1; 3)+
	[2] $C211 (C2, 5)$	(1; 4)+
	[2] $C112_1 (P2_1, 4)$	(1; 2)+
IIa	[2] $P2_12_12_1 (19)$	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P2_12_2 (P2_12_12, 18)$	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P22_12_1 (P2_12_12, 18)$	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P222_1 (17)$	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $C222_1 (\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}) (20)$; [3] $C222_1 (\mathbf{c}' = 3\mathbf{c}) (20)$

Minimal non-isomorphic supergroups

I	[2] $Cmcm (63)$; [2] $Cmce (64)$; [2] $P4_122 (91)$; [2] $P4_12_12 (92)$; [2] $P4_322 (95)$; [2] $P4_32_12 (96)$; [3] $P6_122 (178)$; [3] $P6_522 (179)$; [3] $P6_322 (182)$
II	[2] $F222 (22)$; [2] $P222_1 (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}) (17)$; [2] $C222 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (21)$

$C222$

D_2^6

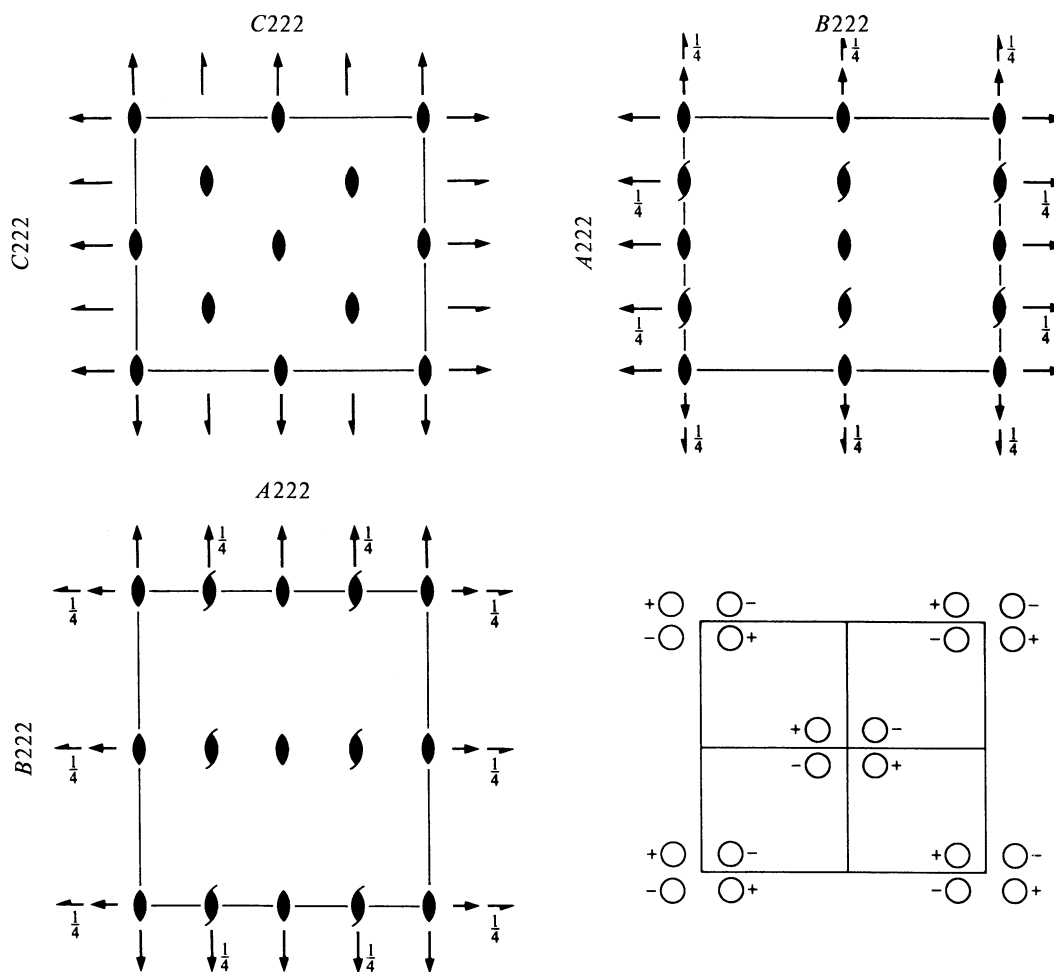
222

Orthorhombic

No. 21

$C222$

Patterson symmetry $Cmmm$



Origin at 222

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) 2 $(0,\frac{1}{2},0) \frac{1}{4},y,0$ (4) 2 $(\frac{1}{2},0,0) x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	(0,0,0)+ $(\frac{1}{2},\frac{1}{2},0)$ +	General:
8 <i>l</i> 1	(1) x,y,z (2) \bar{x},\bar{y},z (3) \bar{x},y,\bar{z} (4) x,\bar{y},\bar{z}	$hkl : h+k=2n$ $hk0 : h+k=2n$ $0kl : k=2n$ $h00 : h=2n$ $h0l : h=2n$ $0k0 : k=2n$
		Special: as above, plus
4 <i>k</i> ..2	$\frac{1}{4},\frac{1}{4},z$ $\frac{3}{4},\frac{1}{4},\bar{z}$	$hk0 : h=2n$
4 <i>j</i> ..2	$0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$	no extra conditions
4 <i>i</i> ..2	$0,0,z$ $0,0,\bar{z}$	no extra conditions
4 <i>h</i> .2.	$0,y,\frac{1}{2}$ $0,\bar{y},\frac{1}{2}$	no extra conditions
4 <i>g</i> .2.	$0,y,0$ $0,\bar{y},0$	no extra conditions
4 <i>f</i> 2..	$x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	no extra conditions
4 <i>e</i> 2..	$x,0,0$ $\bar{x},0,0$	no extra conditions
2 <i>d</i> 222	$0,0,\frac{1}{2}$	no extra conditions
2 <i>c</i> 222	$\frac{1}{2},0,\frac{1}{2}$	no extra conditions
2 <i>b</i> 222	$0,\frac{1}{2},0$	no extra conditions
2 <i>a</i> 222	$0,0,0$	no extra conditions

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0,0,z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at x,0,0

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C121$ ($C2, 5$) (1; 3)+ [2] $C211$ ($C2, 5$) (1; 4)+ [2] $C112$ ($P2, 3$) (1; 2)+
IIa	[2] $P2_12_12$ (18) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $P2_12_2$ ($P222_1, 17$) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $P22_12$ ($P222_1, 17$) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $P222$ (16) 1; 2; 3; 4
IIb	[2] $I2_12_12_1$ ($\mathbf{c}' = 2\mathbf{c}$) (24); [2] $I222$ ($\mathbf{c}' = 2\mathbf{c}$) (23); [2] $C222_1$ ($\mathbf{c}' = 2\mathbf{c}$) (20)

Maximal isomorphic subgroups of lowest index

IIc [2] $C222$ ($\mathbf{c}' = 2\mathbf{c}$) (21); [3] $C222$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (21)

Minimal non-isomorphic supergroups

I	[2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P422$ (89); [2] $P4_22$ (90); [2] $P4_22$ (93); [2] $P4_22_12$ (94); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118); [3] $P622$ (177); [3] $P6_22$ (180); [3] $P6_422$ (181)
II	[2] $F222$ (22); [2] $P222$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (16)

$F 222$

D_2^7

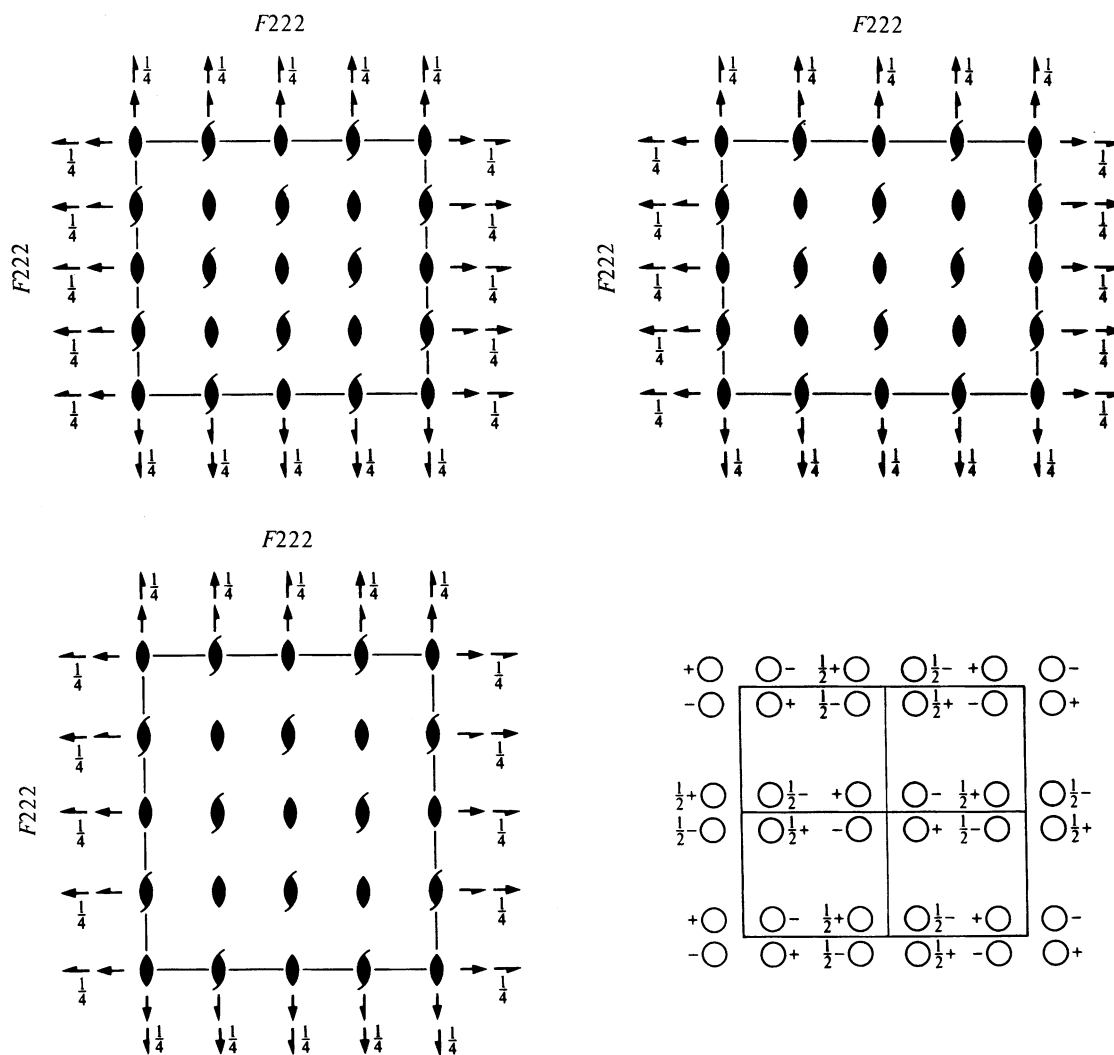
222

Orthorhombic

No. 22

$F 222$

Patterson symmetry $F m m m$



Origin at 222

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1
- (2) $2 \ 0,0,z$
- (3) $2 \ 0,y,0$
- (4) $2 \ x,0,0$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) $t(0, \frac{1}{2}, \frac{1}{2})$
- (2) $2(0,0, \frac{1}{2}) \ 0, \frac{1}{4}, z$
- (3) $2(0, \frac{1}{2}, 0) \ 0,y, \frac{1}{4}$
- (4) $2 \ x, \frac{1}{4}, \frac{1}{4}$

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- (1) $t(\frac{1}{2}, 0, \frac{1}{2})$
- (2) $2(0,0, \frac{1}{2}) \ \frac{1}{4}, 0, z$
- (3) $2 \ \frac{1}{4}, y, \frac{1}{4}$
- (4) $2(\frac{1}{2}, 0, 0) \ x, 0, \frac{1}{4}$

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$
- (2) $2 \ \frac{1}{4}, \frac{1}{4}, z$
- (3) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$
- (4) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, 0$

Maximal isomorphic subgroups of lowest index

Ic [3] $F 222$ ($a' = 3a$ or $b' = 3b$ or $c' = 3c$) (22)

Minimal non-isomorphic supergroups

I [2] $F m m m$ (69); [2] $F d d d$ (70); [2] $I 4 2 2$ (97); [2] $I 4_1 2 2$ (98); [2] $I \bar{4} m 2$ (119); [2] $I \bar{4} c 2$ (120); [3] $F 2 3$ (196)

II [2] $P 222$ ($a' = \frac{1}{2}a, b' = \frac{1}{2}b, c' = \frac{1}{2}c$) (16)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	General:
16	<i>k</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	$hkl : h+k, h+l, k+l = 2n$ $0kl : k, l = 2n$ $h0l : h, l = 2n$ $hk0 : h, k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
8	<i>j</i> 2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$			Special: no extra conditions
8	<i>i</i> .2.	$\frac{1}{4}, y, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \frac{1}{4}$			
8	<i>h</i> ..2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$			
8	<i>g</i> ..2	$0, 0, z$	$0, 0, \bar{z}$			
8	<i>f</i> .2.	$0, y, 0$	$0, \bar{y}, 0$			
8	<i>e</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$			
4	<i>d</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$				
4	<i>c</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$				
4	<i>b</i> 222	$0, 0, \frac{1}{2}$				
4	<i>a</i> 222	$0, 0, 0$				

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at x,0,0

Along [010] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $F112 (C2, 5)$	(1; 2)+
	[2] $F121 (C2, 5)$	(1; 3)+
	[2] $F211 (C2, 5)$	(1; 4)+
IIa	[2] $A222 (C222, 21)$	1; 2; 3; 4; (1; 2; 3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $A222 (C222, 21)$	1; 4; (1; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $B222 (C222, 21)$	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] $B222 (C222, 21)$	1; 3; (1; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $C222 (21)$	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C222 (21)$	1; 2; (1; 2) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] $A2_122 (C222_1, 20)$	1; 2; (1; 2) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $A2_122 (C222_1, 20)$	1; 3; (1; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $B22_12 (C222_1, 20)$	1; 2; (1; 2) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $B22_12 (C222_1, 20)$	1; 4; (1; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $C222_1 (20)$	1; 3; (1; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] $C222_1 (20)$	1; 4; (1; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$
IIb	none	

(Continued on preceding page)

*I*222

D_2^8

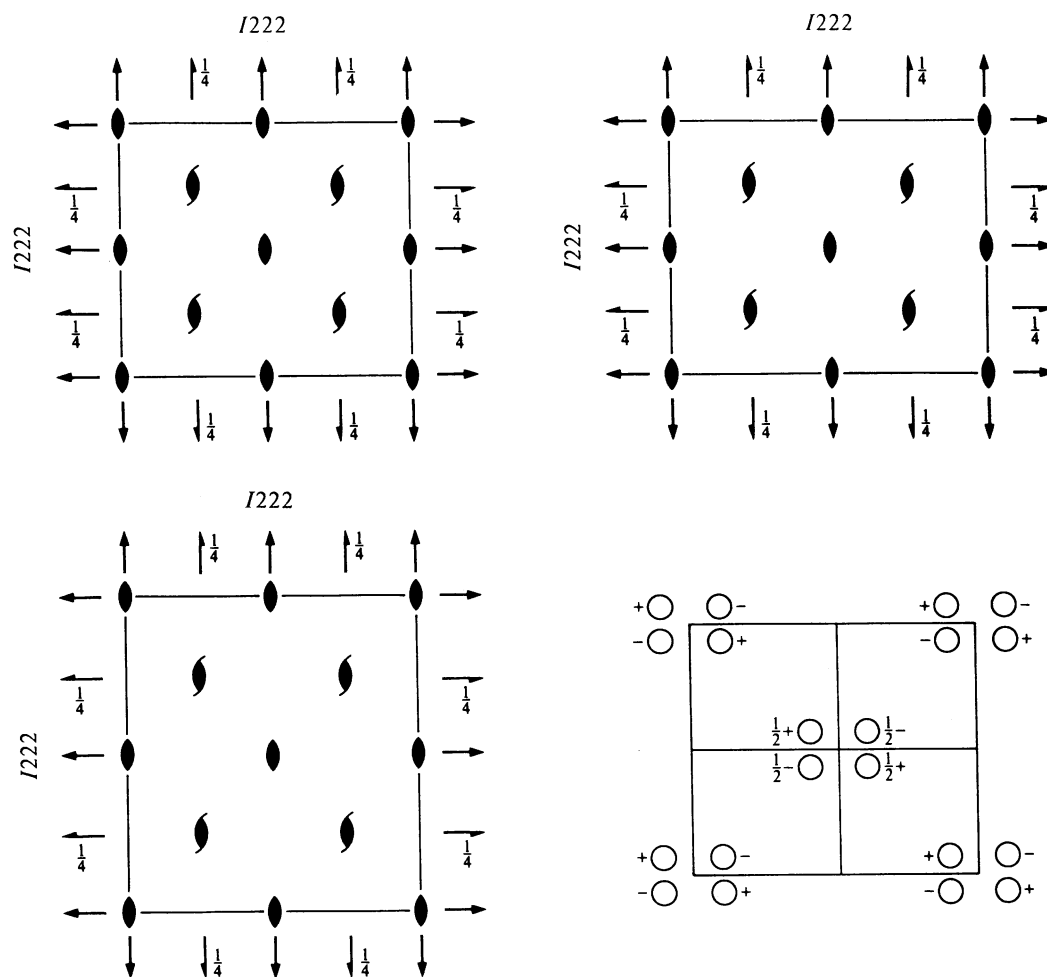
222

Orthorhombic

No. 23

*I*222

Patterson symmetry *I*mmm



Origin at 222

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- (1) 1
- (2) 2 $0,0,z$
- (3) 2 $0,y,0$
- (4) 2 $x,0,0$

For (1/2, 1/2, 1/2)+ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- (2) $2(0,0,\frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$
- (3) $2(0,\frac{1}{2},0) \frac{1}{4}, y, \frac{1}{4}$
- (4) $2(\frac{1}{2},0,0) x, \frac{1}{4}, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		(0,0,0)+	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$			General:
8	<i>k</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	$hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
Special: no extra conditions						
4	<i>j</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$			
4	<i>i</i> ..2	$0, 0, z$	$0, 0, \bar{z}$			
4	<i>h</i> .2.	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$			
4	<i>g</i> .2.	$0, y, 0$	$0, \bar{y}, 0$			
4	<i>f</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$			
4	<i>e</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$			
2	<i>d</i> 222	$0, \frac{1}{2}, 0$				
2	<i>c</i> 222	$0, 0, \frac{1}{2}$				
2	<i>b</i> 222	$\frac{1}{2}, 0, 0$				
2	<i>a</i> 222	$0, 0, 0$				

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x,0,0

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $I112$ (C2, 5)	(1; 2)+
	[2] $I121$ (C2, 5)	(1; 3)+
	[2] $I211$ (C2, 5)	(1; 4)+
IIa	[2] $P2_12_12_1$ (18)	1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P2_12_12_1$ ($P2_12_12_1$, 18)	1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P22_12_1$ ($P2_12_12_1$, 18)	1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P222$ (16)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I222$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (23)

Minimal non-isomorphic supergroups

I [2] $Immm$ (71); [2] $Ibam$ (72); [2] $I422$ (97); [2] $I\bar{4}2m$ (121); [3] $I23$ (197)
II [2] $A222$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (C222, 21); [2] $B222$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (C222, 21); [2] $C222$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (21)

$I2_12_12_1$

D_2^9

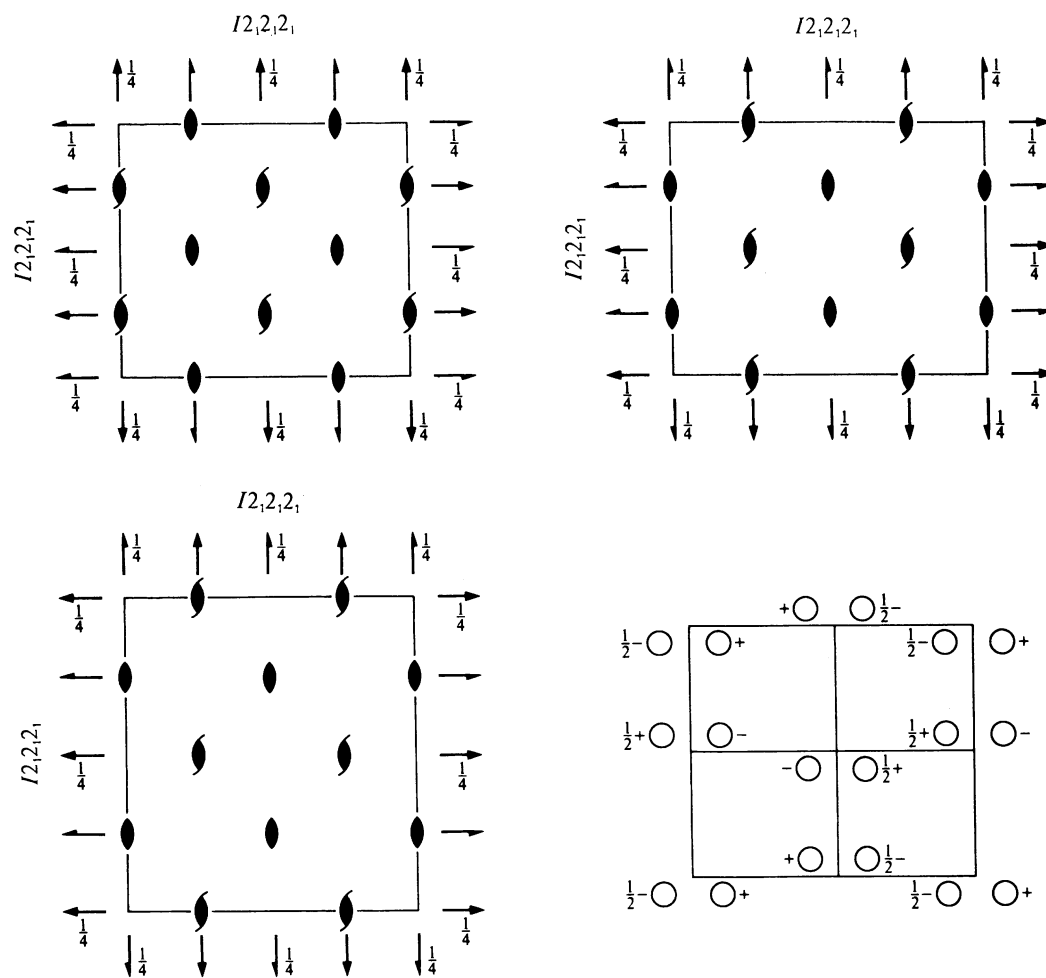
222

Orthorhombic

No. 24

$I2_12_12_1$

Patterson symmetry $Immm$



Origin at midpoint of three non-intersecting pairs of parallel 2 axes

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2(0,0,\frac{1}{2}) \frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0) 0,y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0) x,\frac{1}{4},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2 0,\frac{1}{4},z$ (3) $2 \frac{1}{4},y,0$ (4) $2 x,0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$	General:
8 <i>d</i> 1	(1) x,y,z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
4 <i>c</i> ..2	$0, \frac{1}{4}, z$ $0, \frac{3}{4}, \bar{z} + \frac{1}{2}$	Special: as above, plus $hk0 : h = 2n$
4 <i>b</i> .2.	$\frac{1}{4}, y, 0$ $\frac{1}{4}, \bar{y}, \frac{1}{2}$	$h0l : h = 2n$
4 <i>a</i> 2..	$x, 0, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, 0, \frac{3}{4}$	$0kl : k = 2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $\frac{1}{4}, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{4}, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0, y, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $I112_1 (C2, 5)$ (1; 2)+ [2] $I12_11 (C2, 5)$ (1; 3)+ [2] $I2_111 (C2, 5)$ (1; 4)+
IIa	[2] $P2_12_12_1 (19)$ 1; 2; 3; 4 [2] $P222_1 (17)$ 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ [2] $P22_12 (P222_1, 17)$ 1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ [2] $P2_122 (P222_1, 17)$ 1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
IIb	none

Maximal isomorphic subgroups of lowest index

IIc [3] $I2_12_12_1 (\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}) (24)$

Minimal non-isomorphic supergroups

I	[2] $Ibca (73)$; [2] $Imma (74)$; [2] $I4_122 (98)$; [2] $I\bar{4}2d (122)$; [3] $I2_13 (199)$
II	[2] $A222 (\mathbf{a}' = \frac{1}{2}\mathbf{a}) (C222, 21)$; [2] $B222 (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (C222, 21)$; [2] $C222 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (21)$

$Pmm2$

C_{2v}^1

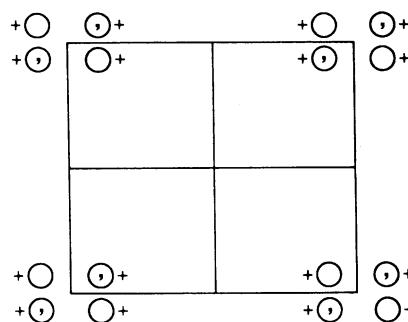
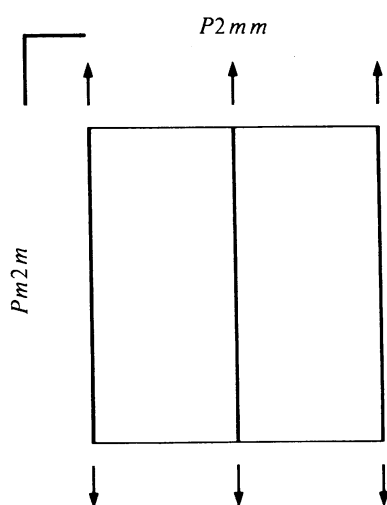
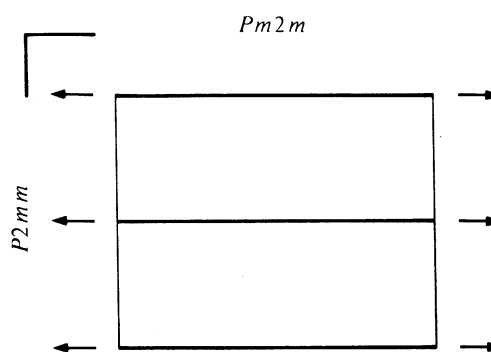
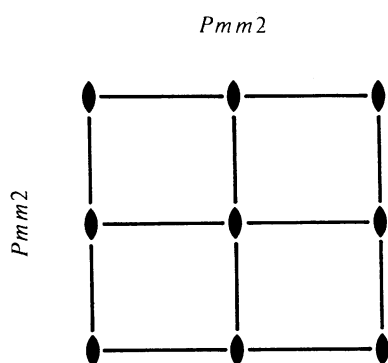
$mm2$

Orthorhombic

No. 25

$Pmm2$

Patterson symmetry $Pmmm$



Origin on $mm2$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>i</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) x,\bar{y},z	(4) \bar{x},y,z	General: no conditions Special: no extra conditions
2 <i>h</i> <i>m</i> . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2 <i>g</i> <i>m</i> . .	$0,y,z$	$0,\bar{y},z$			
2 <i>f</i> . <i>m</i> .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2 <i>e</i> . <i>m</i> .	$x,0,z$	$\bar{x},0,z$			
1 <i>d</i> <i>m m</i> 2	$\frac{1}{2},\frac{1}{2},z$				
1 <i>c</i> <i>m m</i> 2	$\frac{1}{2},0,z$				
1 <i>b</i> <i>m m</i> 2	$0,\frac{1}{2},z$				
1 <i>a</i> <i>m m</i> 2	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, 0, 0

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0, y, 0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm , 6) 1; 3
 [2] $Pm11$ (Pm , 6) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pma2$ ($\mathbf{a}' = 2\mathbf{a}$) (28); [2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2$, 28); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27); [2] $Pmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (26);
 [2] $Pcm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmc2_1$, 26); [2] $Aem2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (39); [2] $Amm2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (38);
 [2] $Bme2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Aem2$, 39); [2] $Bmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Amm2$, 38); [2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35);
 [2] $Fmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)
II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

$Pmc2_1$

C_{2v}^2

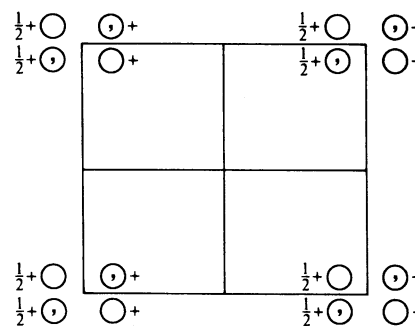
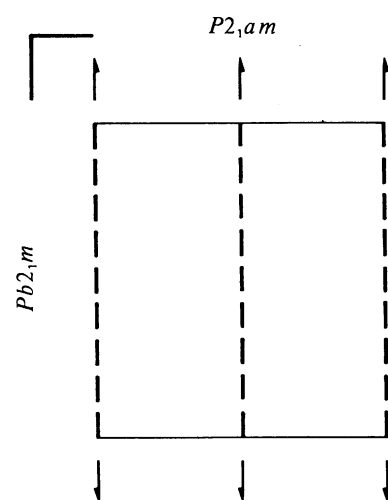
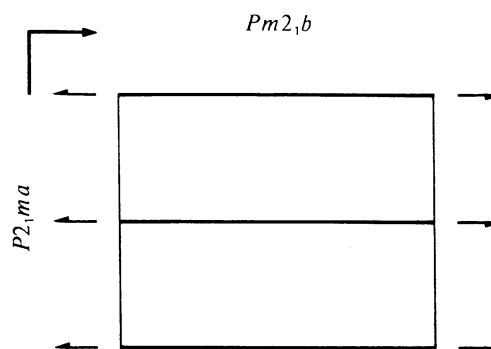
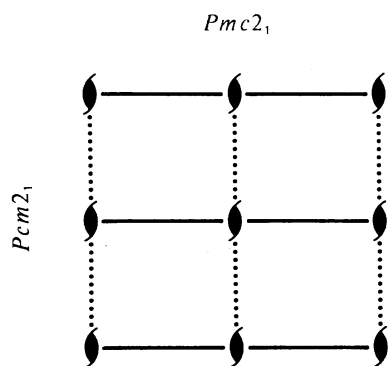
$mm2$

Orthorhombic

No. 26

$Pmc2_1$

Patterson symmetry $Pmmm$



Origin on $mc2_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (3) c $x, 0, z$ (4) m $0, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>c</i> 1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $x, \bar{y}, z + \frac{1}{2}$	(4) \bar{x}, y, z	$h0l : l = 2n$ $00l : l = 2n$
2 <i>b</i> $m..$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z + \frac{1}{2}$			Special: no extra conditions
2 <i>a</i> $m..$	$0, y, z$	$0, \bar{y}, z + \frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1g1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc , 7) 1; 3
 [2] $Pm11$ (Pm , 6) 1; 4
 [2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb [2] $Pmn2_1$ ($\mathbf{a}' = 2\mathbf{a}$) (31); [2] $Pbc2_1$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pca2_1$, 29); [2] $Cmc2_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (36)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmc2_1$ ($\mathbf{a}' = 2\mathbf{a}$) (26); [2] $Pmc2_1$ ($\mathbf{b}' = 2\mathbf{b}$) (26); [3] $Pmc2_1$ ($\mathbf{c}' = 3\mathbf{c}$) (26)

Minimal non-isomorphic supergroups

I [2] $Pmma$ (51); [2] $Pbam$ (55); [2] $Pbcm$ (57); [2] $Pnma$ (62)

II [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Bme2$ ($Aem2$, 39); [2] $Ima2$ (46); [2] $Pmm2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (25)

$Pcc2$

C_{2v}^3

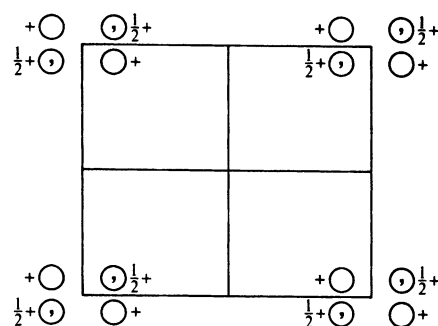
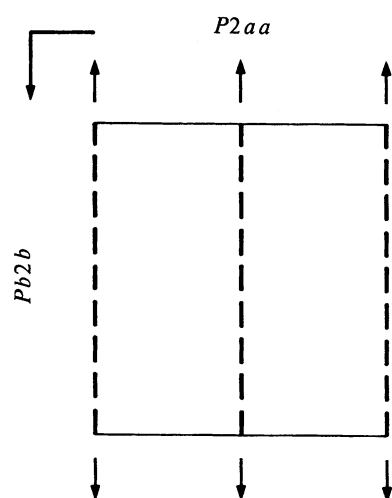
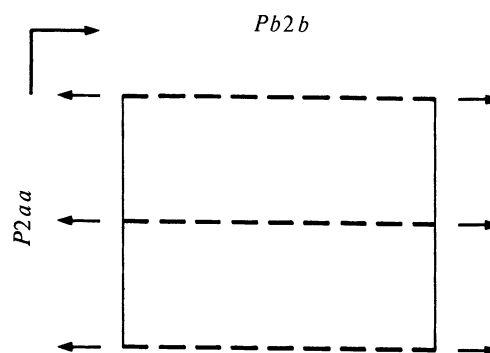
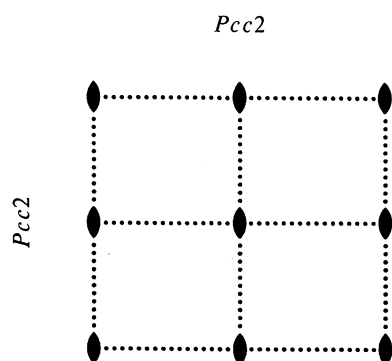
$mm2$

Orthorhombic

No. 27

$Pcc2$

Patterson symmetry $Pmmm$



Origin on $cc2$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) 2 $0,0,z$ (3) c $x,0,z$ (4) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
4 <i>e</i> 1	(1)	x, y, z	(2) \bar{x}, \bar{y}, z	(3) $x, \bar{y}, z + \frac{1}{2}$	(4) $\bar{x}, y, z + \frac{1}{2}$	General: $0kl : l = 2n$ $h0l : l = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : l = 2n$ $hkl : l = 2n$ $hkl : l = 2n$ $hkl : l = 2n$
2 <i>d</i> .. 2		$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			
2 <i>c</i> .. 2		$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$			
2 <i>b</i> .. 2		$0, \frac{1}{2}, z$	$0, \frac{1}{2}, z + \frac{1}{2}$			
2 <i>a</i> .. 2		$0, 0, z$	$0, 0, z + \frac{1}{2}$			

Symmetry of special projections

Along $[001]$ $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along $[010]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc , 7) 1; 3
 [2] $Pc11$ (Pc , 7) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pcn2$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pnc2$, 30); [2] $Pnc2$ ($\mathbf{b}' = 2\mathbf{b}$) (30); [2] $Ccc2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (37)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pcc2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (27); [3] $Pcc2$ ($\mathbf{c}' = 3\mathbf{c}$) (27)

Minimal non-isomorphic supergroups

I [2] $Pccm$ (49); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $P4_2cm$ (101); [2] $P4cc$ (103); [2] $P\bar{4}c2$ (116)

II [2] $Ccc2$ (37); [2] $Aem2$ (39); [2] $Bme2$ ($Aem2$, 39); [2] $Iba2$ (45); [2] $Pmm2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (25)

$Pma2$

C_{2v}^4

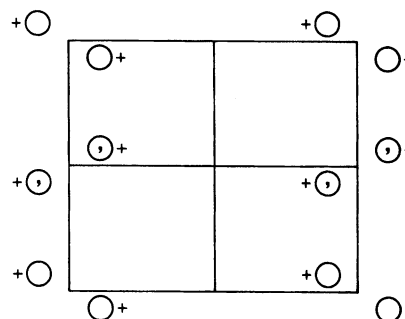
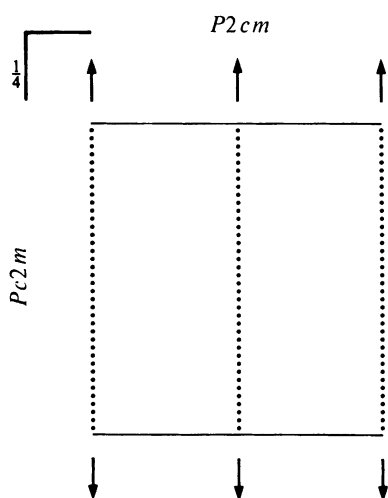
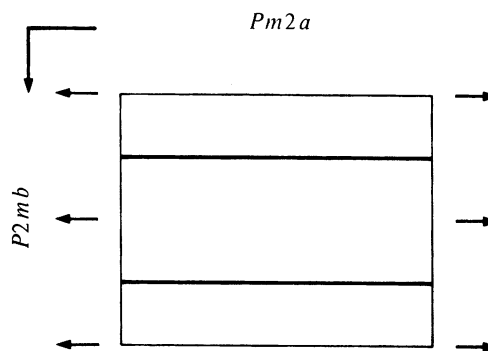
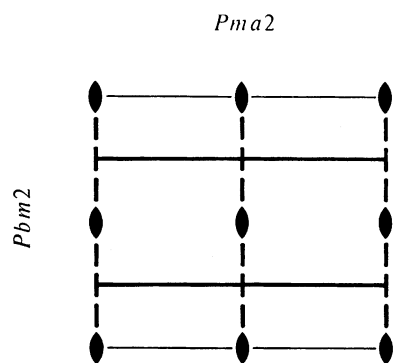
$mm2$

Orthorhombic

No. 28

$Pma2$

Patterson symmetry $Pmmm$



Origin on $1a2$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2 \ 0,0,z$ (3) $a \ x,0,z$ (4) $m \ \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>d</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	General: $h0l : h = 2n$ $h00 : h = 2n$ Special: as above, plus no extra conditions
2 <i>c</i> $m..$	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			$hkl : h = 2n$
2 <i>b</i> $..2$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$			$hkl : h = 2n$
2 <i>a</i> $..2$	$0,0,z$	$\frac{1}{2},0,z$			$hkl : h = 2n$

Symmetry of special projections

Along [001] $p2mg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0,0,z

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc , 7) 1; 3
[2] $Pm11$ (Pm , 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pba2$ ($\mathbf{b}' = 2\mathbf{b}$) (32); [2] $Pmn2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (31); [2] $Pcn2$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnc2$, 30); [2] $Pca2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (29);
[2] $Aea2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (41); [2] $Ama2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (40)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pma2$ ($\mathbf{b}' = 2\mathbf{b}$) (28); [2] $Pma2$ ($\mathbf{c}' = 2\mathbf{c}$) (28); [3] $Pma2$ ($\mathbf{a}' = 3\mathbf{a}$) (28)

Minimal non-isomorphic supergroups

I [2] $Pccm$ (49); [2] $Pmma$ (51); [2] $Pmna$ (53); [2] $Pbcm$ (57)

II [2] $Cmm2$ (35); [2] $Bme2$ ($Aem2$, 39); [2] $Ama2$ (40); [2] $Ima2$ (46); [2] $Pmm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (25)

$Pca2_1$

C_{2v}^5

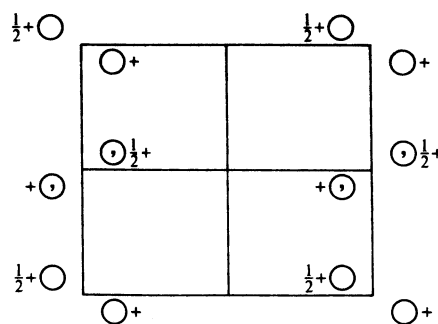
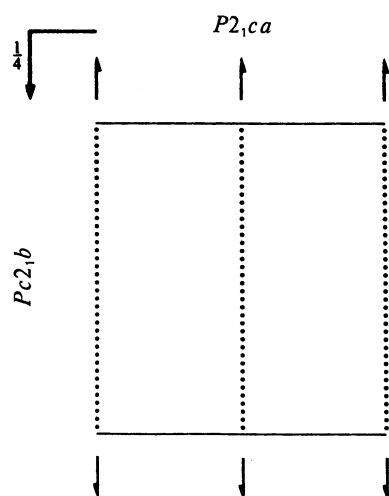
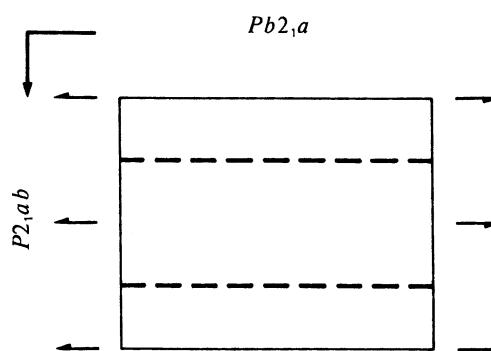
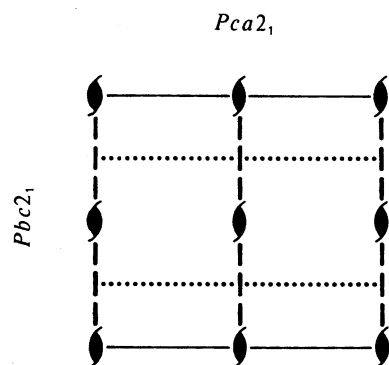
$mm2$

Orthorhombic

No. 29

$Pca2_1$

Patterson symmetry $Pmmm$



Origin on $1a2_1$

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq 1$; $0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (3) a $x, 0, z$ (4) c $\frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $x + \frac{1}{2}, \bar{y}, z$	(4) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	$0kl : l = 2n$ $h0l : h = 2n$ $h00 : h = 2n$ $00l : l = 2n$

Symmetry of special projections

Along [001] $p2mg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11g$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc , 7) 1; 3
 [2] $Pc11$ (Pc , 7) 1; 4
 [2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb [2] $Pna2_1$ ($\mathbf{b}' = 2\mathbf{b}$) (33)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pca2_1$ ($\mathbf{b}' = 2\mathbf{b}$) (29); [3] $Pca2_1$ ($\mathbf{a}' = 3\mathbf{a}$) (29); [3] $Pca2_1$ ($\mathbf{c}' = 3\mathbf{c}$) (29)

Minimal non-isomorphic supergroups

I [2] $Pcca$ (54); [2] $Pbcm$ (57); [2] $Pbcn$ (60); [2] $Pbca$ (61)

II [2] $Ccm2_1$ ($Cmc2_1$, 36); [2] $Bme2$ ($Aem2$, 39); [2] $Aea2$ (41); [2] $Iba2$ (45); [2] $Pcm2_1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmc2_1$, 26);
 [2] $Pma2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (28)

$Pnc2$

C_{2v}^6

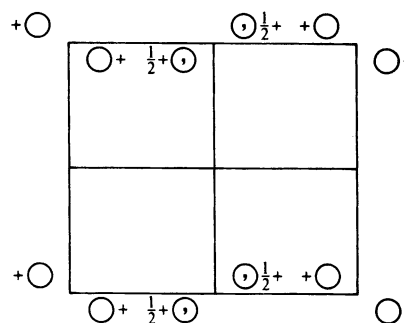
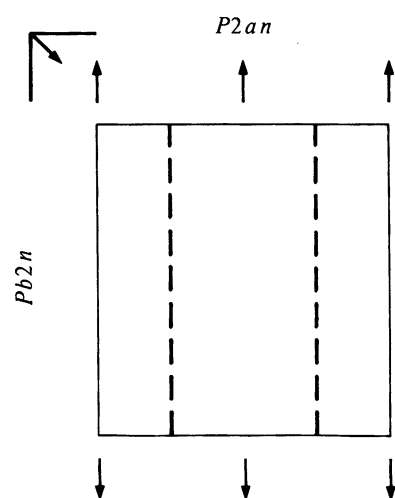
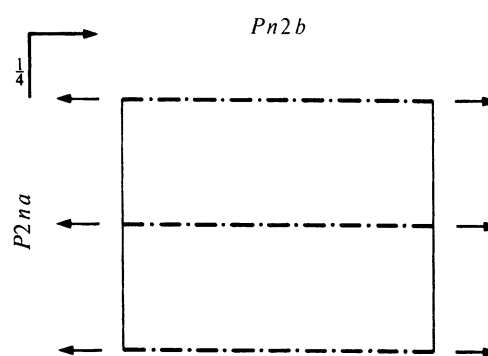
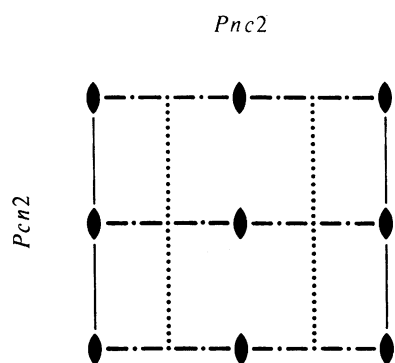
$mm2$

Orthorhombic

No. 30

$Pnc2$

Patterson symmetry $Pmmm$



Origin on $n12$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- (1) 1 (2) $2 \ 0,0,z$ (3) $c \ x, \frac{1}{4}, z$ (4) $n(0, \frac{1}{2}, \frac{1}{2}) \ 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl : k+l=2n$ $h0l : l=2n$ $0k0 : k=2n$ $00l : l=2n$
					Special: as above, plus
2 <i>b</i> ..2	$\frac{1}{2},0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			$hkl : k+l=2n$
2 <i>a</i> ..2	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{2}$			$hkl : k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x,0,0

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc , 7) 1; 3
 [2] $Pn11$ (Pc , 7) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pnn2$ ($\mathbf{a}' = 2\mathbf{a}$) (34)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pnc2$ ($\mathbf{a}' = 2\mathbf{a}$) (30); [3] $Pnc2$ ($\mathbf{b}' = 3\mathbf{b}$) (30); [3] $Pnc2$ ($\mathbf{c}' = 3\mathbf{c}$) (30)

Minimal non-isomorphic supergroups

I [2] $Pban$ (50); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pbcn$ (60)

II [2] $Ccc2$ (37); [2] $Amm2$ (38); [2] $Bbe2$ ($Aea2$, 41); [2] $Ima2$ (46); [2] $Pcc2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (27); [2] $Pbm2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pma2$, 28)

$Pmn2_1$

C_{2v}^7

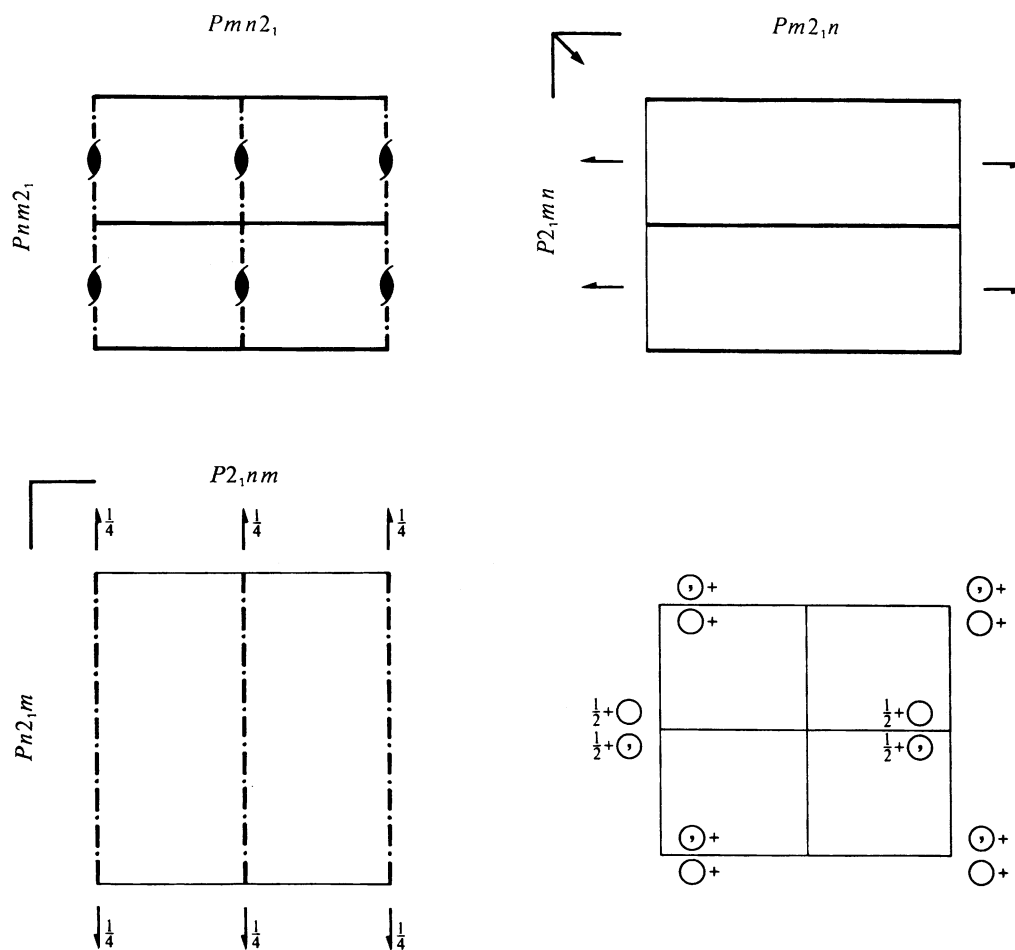
$mm2$

Orthorhombic

No. 31

$Pmn2_1$

Patterson symmetry $Pmmm$



Origin on $mn1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, 0, \frac{1}{2}) \frac{1}{4}, 0, z$ (3) $n(\frac{1}{2}, 0, \frac{1}{2}) x, 0, z$ (4) $m 0, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>b</i> 1	(1) x,y,z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(4) \bar{x}, y, z	$h0l : h + l = 2n$ $h00 : h = 2n$ $00l : l = 2n$
					Special: no extra conditions
2 <i>a</i> $m..$	$0,y,z$	$\frac{1}{2}, \bar{y}, z + \frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $\frac{1}{4}, 0, z$

Along [100] $p1g1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $c11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I [2] $P1n1$ (Pc , 7) 1; 3
 [2] $Pm11$ (Pm , 6) 1; 4
 [2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb [2] $Pbn2_1$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pna2_1$, 33)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmn2_1$ ($\mathbf{b}' = 2\mathbf{b}$) (31); [3] $Pmn2_1$ ($\mathbf{a}' = 3\mathbf{a}$) (31); [3] $Pmn2_1$ ($\mathbf{c}' = 3\mathbf{c}$) (31)

Minimal non-isomorphic supergroups

I [2] $Pmna$ (53); [2] $Pnmm$ (58); [2] $Pmmn$ (59); [2] $Pnma$ (62)

II [2] $Cmc2_1$ (36); [2] $Bmm2$ ($Amm2$, 38); [2] $Ama2$ (40); [2] $Imm2$ (44); [2] $Pmc2_1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (26); [2] $Pma2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (28)

*Pba*2

C_{2v}^8

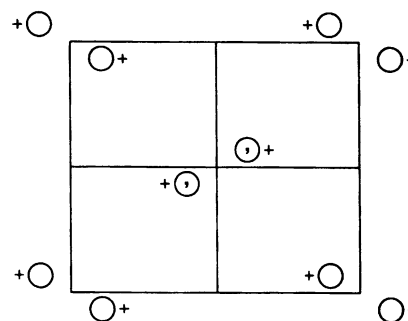
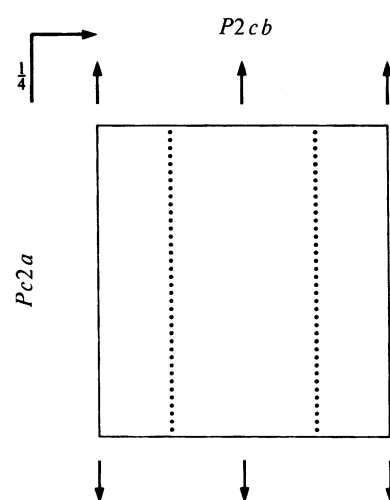
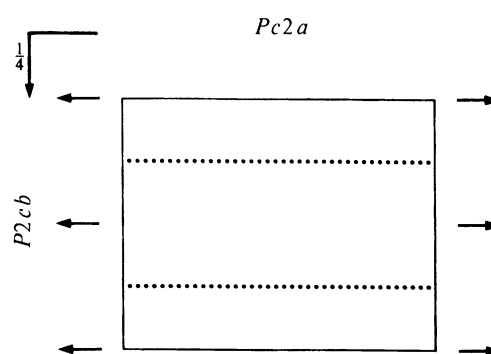
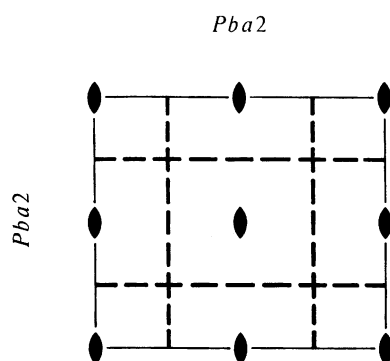
*mm*2

Orthorhombic

No. 32

*Pba*2

Patterson symmetry *Pmmm*



Origin on 112

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) 2 $0,0,z$ (3) *a* $x, \frac{1}{4}, z$ (4) *b* $\frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl : k = 2n$ $h0l : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$
2 <i>b</i> ..2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			Special: as above, plus $hkl : h + k = 2n$
2 <i>a</i> ..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0,0,z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc , 7) 1; 3
[2] $Pb11$ (Pc , 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pnn2$ ($\mathbf{c}' = 2\mathbf{c}$) (34); [2] $Pna2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (33); [2] $Pbn2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pna2_1$, 33)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pba2$ ($\mathbf{c}' = 2\mathbf{c}$) (32); [3] $Pba2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (32)

Minimal non-isomorphic supergroups

I [2] $Pban$ (50); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $P4bm$ (100); [2] $P4_2bc$ (106); [2] $P\bar{4}b2$ (117)

II [2] $Cmm2$ (35); [2] $Aea2$ (41); [2] $Bbe2$ ($Aea2$, 41); [2] $Iba2$ (45); [2] $Pbm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pma2$, 28); [2] $Pma2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (28)

$Pna2_1$

C_{2v}^9

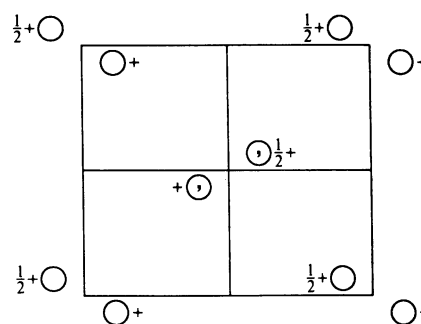
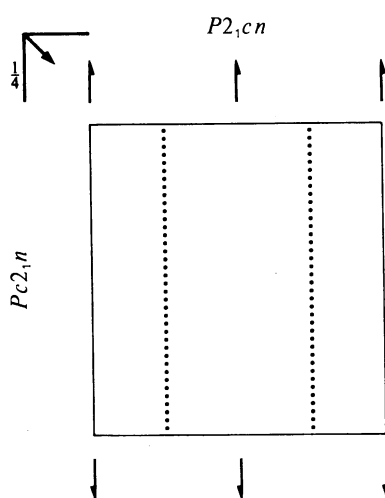
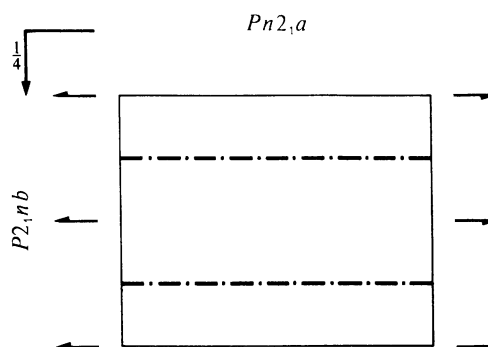
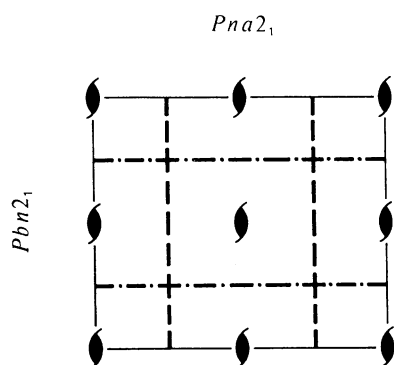
$mm2$

Orthorhombic

No. 33

$Pna2_1$

Patterson symmetry $Pmmm$



Origin on 112_1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (3) a $x, \frac{1}{4}, z$ (4) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>a</i> 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl : k+l=2n$ $h0l : h=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0,0,z

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{4}, 0$

Along [010] $p11g$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc , 7) 1; 3
 [2] $Pn11$ (Pc , 7) 1; 4
 [2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pna2_1$ ($\mathbf{a}' = 3\mathbf{a}$) (33); [3] $Pna2_1$ ($\mathbf{b}' = 3\mathbf{b}$) (33); [3] $Pna2_1$ ($\mathbf{c}' = 3\mathbf{c}$) (33)

Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pccn$ (56); [2] $Pbcn$ (60); [2] $Pnma$ (62)

II [2] $Ccm2_1$ ($Cmc2_1$, 36); [2] $Ama2$ (40); [2] $Bbe2$ ($Aea2$, 41); [2] $Ima2$ (46); [2] $Pca2_1$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (29);
 [2] $Pnm2_1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmn2_1$, 31); [2] $Pba2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (32)

$Pnn2$

C_{2v}^{10}

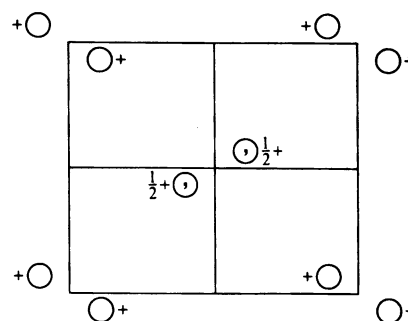
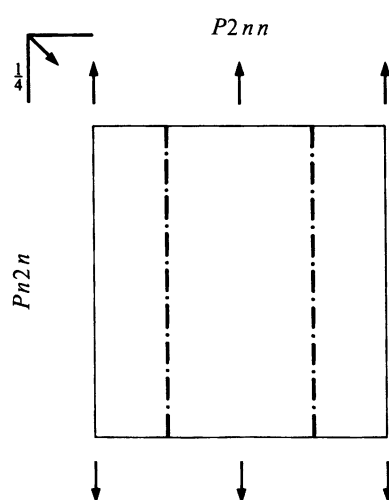
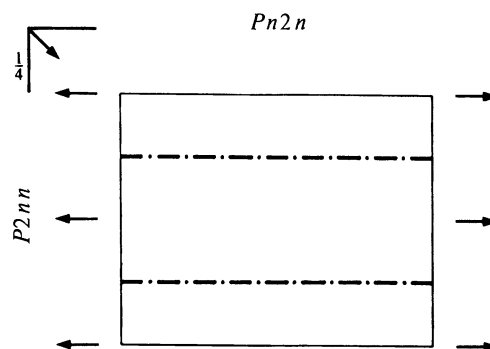
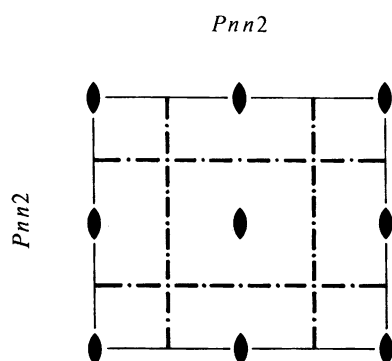
$mm2$

Orthorhombic

No. 34

$Pnn2$

Patterson symmetry $Pmmm$



Origin on 112

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) 2 $0,0,z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$Ok\bar{l} : k+l=2n$ $h0l : h+l=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
					Special: as above, plus
2 <i>b</i> ..2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			$hkl : h+k+l=2n$
2 <i>a</i> ..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			$hkl : h+k+l=2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along [010] $c11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1n1$ (Pc , 7) 1; 3
 [2] $Pn11$ (Pc , 7) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Fdd2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (43)

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnn2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (34); [3] $Pnn2$ ($\mathbf{c}' = 3\mathbf{c}$) (34)

Minimal non-isomorphic supergroups

I [2] $Pnnn$ (48); [2] $Pnna$ (52); [2] $Pnmm$ (58); [2] $P4_2nm$ (102); [2] $P4nc$ (104); [2] $P\bar{4}n2$ (118)

II [2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Bbm2$ ($Ama2$, 40); [2] $Imm2$ (44); [2] $Pnc2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (30); [2] $Pcn2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pnc2$, 30); [2] $Pba2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (32)

$Cmm2$

C_{2v}^{11}

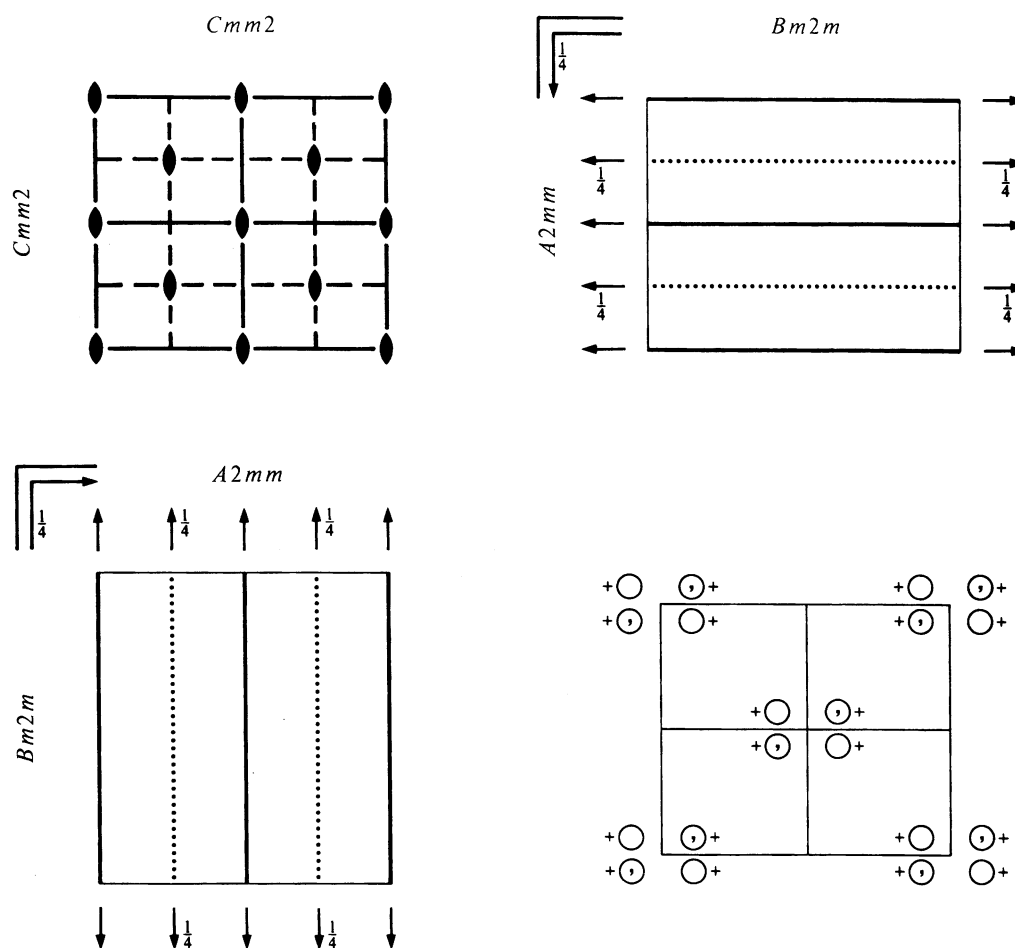
$mm2$

Orthorhombic

No. 35

$Cmm2$

Patterson symmetry $Cmmm$



Origin on $mm2$

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+ $(\frac{1}{2},\frac{1}{2},0)$ +				General:
8 <i>f</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) x,\bar{y},z	(4) \bar{x},y,z	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$
4 <i>e</i> $m..$	$0,y,z$	$0,\bar{y},z$			Special: as above, plus no extra conditions
4 <i>d</i> $.m.$	$x,0,z$	$\bar{x},0,z$			no extra conditions
4 <i>c</i> $..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			$hkl : h=2n$
2 <i>b</i> $mm2$	$0,\frac{1}{2},z$				no extra conditions
2 <i>a</i> $mm2$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C1m1$ (Cm , 8)	(1; 3)+
	[2] $Cm11$ (Cm , 8)	(1; 4)+
	[2] $C112$ ($P2$, 3)	(1; 2)+
IIa	[2] $Pba2$ (32)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbm2$ ($Pma2$, 28)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pma2$ (28)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmm2$ (25)	1; 2; 3; 4
IIb	[2] $Ima2$ ($\mathbf{c}' = 2\mathbf{c}$) (46); [2] $Ibm2$ ($\mathbf{c}' = 2\mathbf{c}$) ($Ima2$, 46); [2] $Iba2$ ($\mathbf{c}' = 2\mathbf{c}$) (45); [2] $Imm2$ ($\mathbf{c}' = 2\mathbf{c}$) (44); [2] $Ccc2$ ($\mathbf{c}' = 2\mathbf{c}$) (37); [2] $Cmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (36); [2] $Ccm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Cmc2_1$, 36)	

Maximal isomorphic subgroups of lowest index

IIc [2] $Cmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (35); [3] $Cmm2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (35)

Minimal non-isomorphic supergroups

I	[2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2_1m$ (113); [3] $P6mm$ (183)
II	[2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (25)

$Cmc2_1$

C_{2v}^{12}

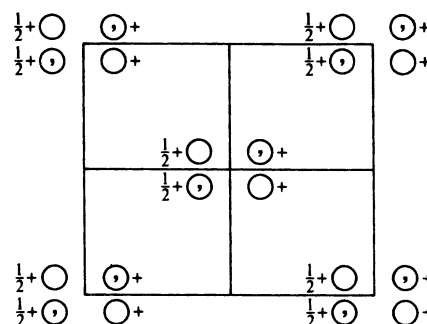
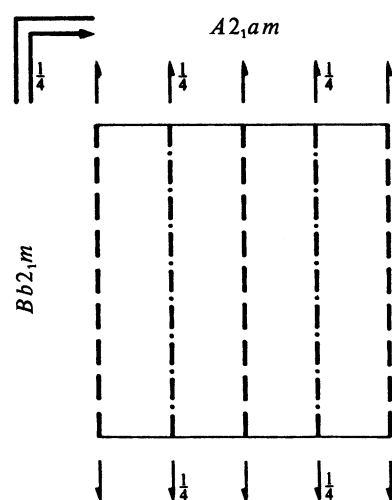
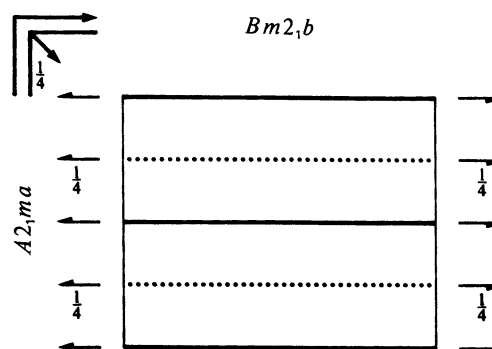
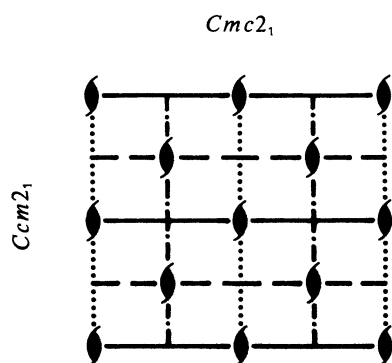
$mm2$

Orthorhombic

No. 36

$Cmc2_1$

Patterson symmetry $Cmmm$



Origin on $mc2_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2(0,0,\frac{1}{2})$ (3) c (4) m

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,0,\frac{1}{2})$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ (4) b

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$

Reflection conditions

General:

8 b 1 (1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $x,\bar{y},z+\frac{1}{2}$ (4) \bar{x},y,z

$hkl : h+k=2n$

$0kl : k=2n$

$h0l : h,l=2n$

$hk0 : h+k=2n$

$h00 : h=2n$

$0k0 : k=2n$

$00l : l=2n$

Special: no extra conditions

4 a $m..$ $0,y,z$ $0,\bar{y},z+\frac{1}{2}$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0,0,z$

Along [100] $p1g1$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x,0,0$

Along [010] $p11m$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C1c1$ (Cc , 9) (1; 3)+

[2] $Cm11$ (Cm , 8) (1; 4)+

[2] $C112_1$ ($P2_1$, 4) (1; 2)+

IIa [2] $Pbn2_1$ ($Pna2_1$, 33) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$

[2] $Pmn2_1$ (31) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$

[2] $Pbc2_1$ ($Pca2_1$, 29) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$

[2] $Pmc2_1$ (26) 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmc2_1$ ($\mathbf{a}' = 3\mathbf{a}$) (36); [3] $Cmc2_1$ ($\mathbf{b}' = 3\mathbf{b}$) (36); [3] $Cmc2_1$ ($\mathbf{c}' = 3\mathbf{c}$) (36)

Minimal non-isomorphic supergroups

I [2] $Cmcm$ (63); [2] $Cmce$ (64); [3] $P6_3cm$ (185); [3] $P6_3mc$ (186)

II [2] $Fmm2$ (42); [2] $Pmc2_1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (26); [2] $Cmm2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (35)

$Ccc2$

C_{2v}^{13}

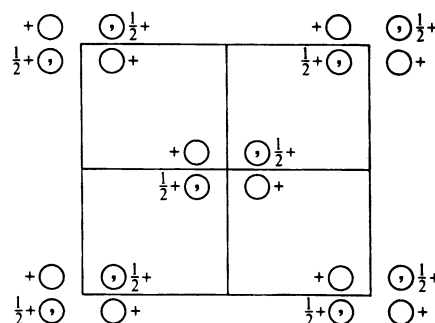
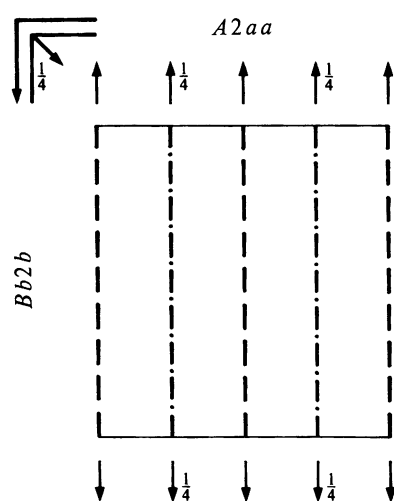
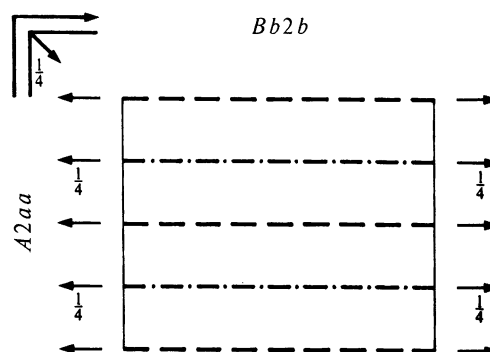
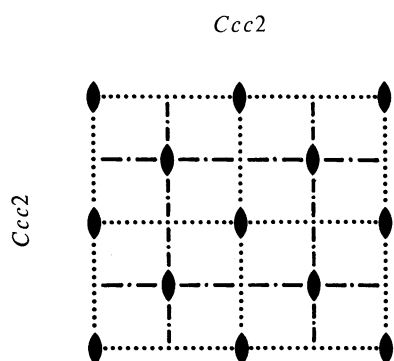
$mm2$

Orthorhombic

No. 37

$Ccc2$

Patterson symmetry $Cmmm$



Origin on $cc2$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2 \ 0,0,z$ (3) $c \ x,0,z$ (4) $c \ 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2 \ \frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2}) \ x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2}) \ \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8 <i>d</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z+\frac{1}{2}$	$hkl : h+k=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
4 <i>c</i> ..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$			$hkl : k+l=2n$
4 <i>b</i> ..2	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$			$hkl : l=2n$
4 <i>a</i> ..2	$0,0,z$	$0,0,z+\frac{1}{2}$			$hkl : l=2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at x,0,0

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C1c1$ (Cc , 9)	(1; 3)+
	[2] $Cc11$ (Cc , 9)	(1; 4)+
	[2] $C112$ ($P2$, 3)	(1; 2)+
IIa	[2] $Pnn2$ (34)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnc2$ (30)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcn2$ ($Pnc2$, 30)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcc2$ (27)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ccc2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (37); [3] $Ccc2$ ($\mathbf{c}' = 3\mathbf{c}$) (37)

Minimal non-isomorphic supergroups

I	[2] $Cccm$ (66); [2] $Ccce$ (68); [2] $P4cc$ (103); [2] $P4nc$ (104); [2] $P4_2mc$ (105); [2] $P4_2bc$ (106); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2_1c$ (114); [3] $P6cc$ (184)
II	[2] $Fmm2$ (42); [2] $Pcc2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (27); [2] $Cmm2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (35)

*Amm*2

C_{2v}^{14}

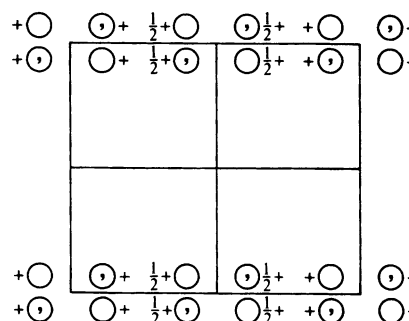
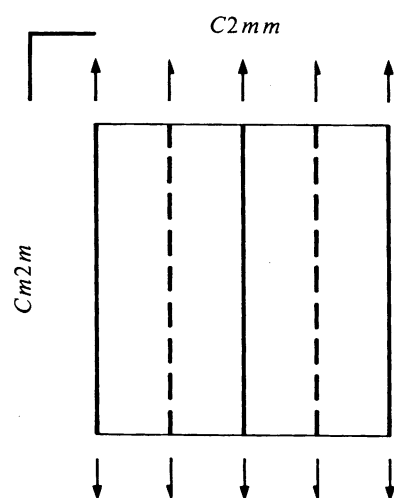
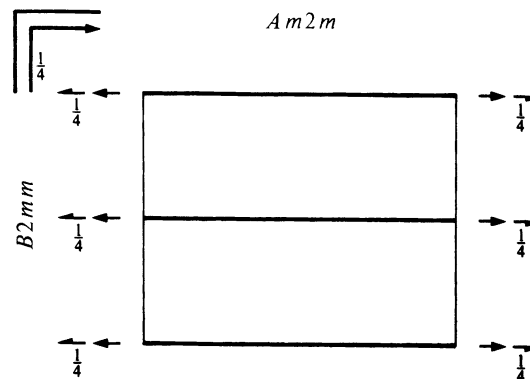
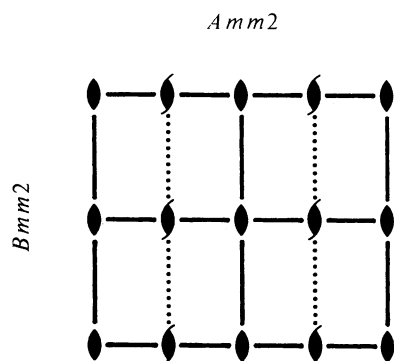
*mm*2

Orthorhombic

No. 38

*Amm*2

Patterson symmetry *Ammm* (*Cmmm*)



Origin on *mm*2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) 2 $0,0,z$ (3) *m* $x,0,z$ (4) *m* $0,y,z$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) *t* $(0, \frac{1}{2}, \frac{1}{2})$ (2) 2 $(0,0, \frac{1}{2})$ $0, \frac{1}{4}, z$ (3) *c* $x, \frac{1}{4}, z$ (4) *n* $(0, \frac{1}{2}, \frac{1}{2})$ $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$			General:
8 <i>f</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) x,\bar{y},z	(4) \bar{x},y,z	$hkl : k+l=2n$ $0kl : k+l=2n$ $h0l : l=2n$ $hk0 : k=2n$ $0k0 : k=2n$ $00l : l=2n$
4 <i>e</i> <i>m</i> . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
4 <i>d</i> <i>m</i> . .	$0,y,z$	$0,\bar{y},z$			
4 <i>c</i> . <i>m</i> .	$x,0,z$	$\bar{x},0,z$			
2 <i>b</i> <i>m m</i> 2	$\frac{1}{2},0,z$				
2 <i>a</i> <i>m m</i> 2	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x,0,0

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $A1m1$ (Cm , 8)	(1; 3)+
	[2] $Am11$ (Pm , 6)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pnm2_1$ ($Pmn2_1$, 31)	1; 3; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $Pnc2$ (30)	1; 2; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmc2_1$ (26)	1; 4; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmm2$ (25)	1; 2; 3; 4
IIb	[2] $Ima2$ ($\mathbf{a}' = 2\mathbf{a}$) (46); [2] $Imm2$ ($\mathbf{a}' = 2\mathbf{a}$) (44); [2] $Ama2$ ($\mathbf{a}' = 2\mathbf{a}$) (40)	

Maximal isomorphic subgroups of lowest index

IIc [2] $Amm2$ ($\mathbf{a}' = 2\mathbf{a}$) (38); [3] $Amm2$ ($\mathbf{b}' = 3\mathbf{b}$) (38); [3] $Amm2$ ($\mathbf{c}' = 3\mathbf{c}$) (38)

Minimal non-isomorphic supergroups

I	[2] $Cmcm$ (63); [2] $Cmmm$ (65); [3] $P\bar{6}m2$ (187); [3] $P\bar{6}2m$ (189)
II	[2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (25)

Aem2

C_{2v}^{15}

mm2

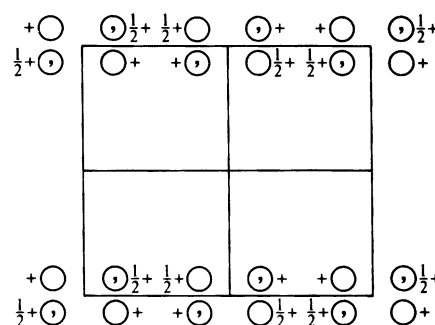
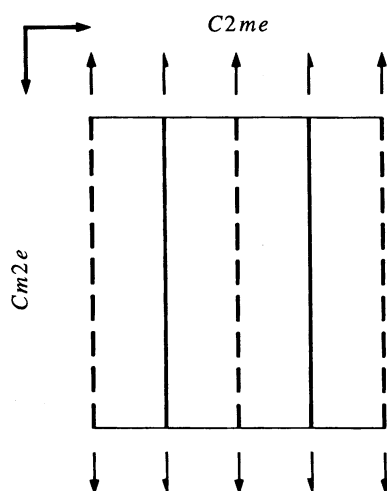
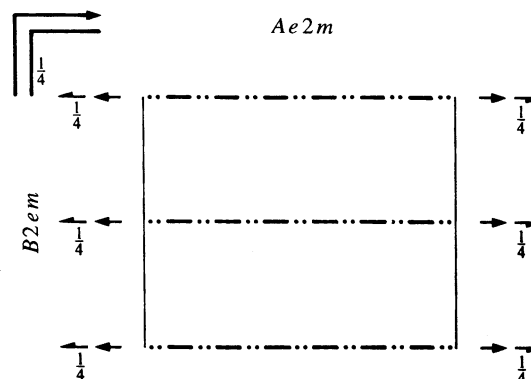
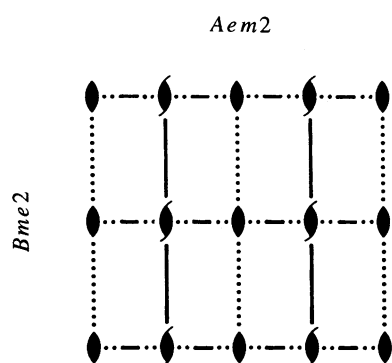
Orthorhombic

No. 39

Aem2

Patterson symmetry *Ammm* (*Cmmm*)

Former space-group symbol *Abm2*; cf. Chapter 1.3



Origin on *ec2*

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) 2 $0,0,z$ (3) *m* $x, \frac{1}{4}, z$ (4) *b* $0,y,z$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) *t* $(0, \frac{1}{2}, \frac{1}{2})$ (2) 2 $(0,0, \frac{1}{2})$ $0, \frac{1}{4}, z$ (3) *c* $x,0,z$ (4) *c* $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+			General:
8 <i>d</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $x, \bar{y} + \frac{1}{2}, z$	(4) $\bar{x}, y + \frac{1}{2}, z$	$hkl : k + l = 2n$ $0kl : k, l = 2n$ $h0l : l = 2n$ $hk0 : k = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
4 <i>c</i> . <i>m</i> .	$x, \frac{1}{4}, z$	$\bar{x}, \frac{3}{4}, z$			Special: as above, plus no extra conditions
4 <i>b</i> . . 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, \frac{1}{2}, z$			$hkl : k = 2n$
4 <i>a</i> . . 2	$0, 0, z$	$0, \frac{1}{2}, z$			$hkl : k = 2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0, 0, z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $A1m1$ (Cm , 8)	(1; 3)+
	[2] $Ae11$ (Pc , 7)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 4; (2; 3) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $Pbm2$ ($Pma2$, 28)	1; 2; 3; 4
	[2] $Pcc2$ (27)	1; 2; (3; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $Pcm2_1$ ($Pmc2_1$, 26)	1; 3; (2; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
IIb	[2] $Ibm2$ ($\mathbf{a}' = 2\mathbf{a}$) ($Ima2$, 46); [2] $Iba2$ ($\mathbf{a}' = 2\mathbf{a}$) (45); [2] $Aea2$ ($\mathbf{a}' = 2\mathbf{a}$) (41)	

Maximal isomorphic subgroups of lowest index

IIc [2] $Aem2$ ($\mathbf{a}' = 2\mathbf{a}$) (39); [3] $Aem2$ ($\mathbf{b}' = 3\mathbf{b}$) (39); [3] $Aem2$ ($\mathbf{c}' = 3\mathbf{c}$) (39)

Minimal non-isomorphic supergroups

I	[2] $Cmce$ (64); [2] $Cmme$ (67)
II	[2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (25)

*Ama*2

C_{2v}^{16}

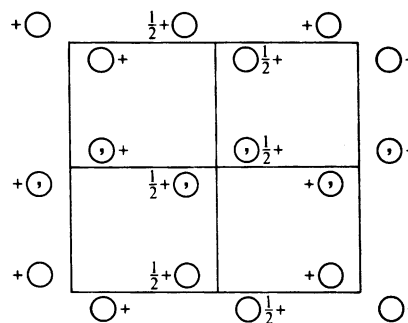
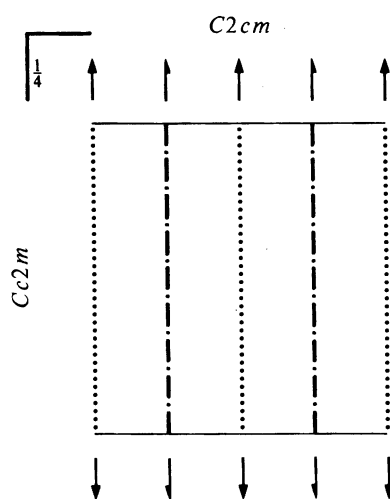
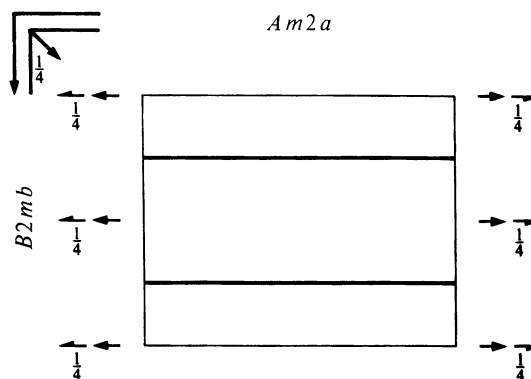
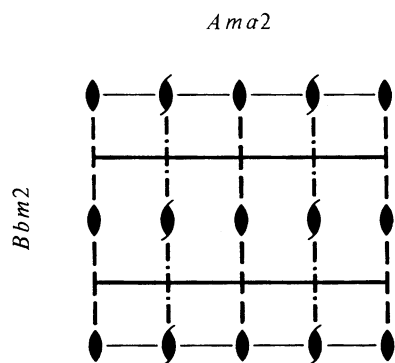
*mm*2

Orthorhombic

No. 40

*Ama*2

Patterson symmetry *Ammm* (*Cmmm*)



Origin on 1*a*2

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

For (0,0,0)+ set

- (1) 1 (2) 2 $0,0,z$ (3) *a* $x,0,z$ (4) *m* $\frac{1}{4},y,z$

For $(0, \frac{1}{2}, \frac{1}{2})$ + set

- (1) *t* $(0, \frac{1}{2}, \frac{1}{2})$ (2) 2 $(0,0, \frac{1}{2})$ $0, \frac{1}{4}, z$ (3) *n* $(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ (4) *n* $(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+			General:
8 c 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x + \frac{1}{2}, \bar{y}, z$	(4) $\bar{x} + \frac{1}{2}, y, z$	$hkl : k + l = 2n$ $0kl : k + l = 2n$ $h0l : h, l = 2n$ $hk0 : k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
4 b m . .	$\frac{1}{4}, y, z$	$\frac{3}{4}, \bar{y}, z$			Special: as above, plus no extra conditions
4 a . . 2	0,0,z	$\frac{1}{2}, 0, z$			$hkl : h = 2n$

Symmetry of special projections

Along [001] $p2mg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $A1a1$ (Cc , 9)	(1; 3)+
	[2] $Am11$ (Pm , 6)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pnn2$ (34)	1; 2; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $Pna2_1$ (33)	1; 3; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmn2_1$ (31)	1; 4; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] $Pma2$ (28)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ama2$ ($\mathbf{a}' = 3\mathbf{a}$) (40); [3] $Ama2$ ($\mathbf{b}' = 3\mathbf{b}$) (40); [3] $Ama2$ ($\mathbf{c}' = 3\mathbf{c}$) (40)

Minimal non-isomorphic supergroups

I [2] $Cmcm$ (63); [2] $Cccm$ (66); [3] $P\bar{6}c2$ (188); [3] $P\bar{6}2c$ (190)
II [2] $Fmm2$ (42); [2] $Pma2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (28); [2] $Amm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (38)

Aea2

C_{2v}^{17}

mm2

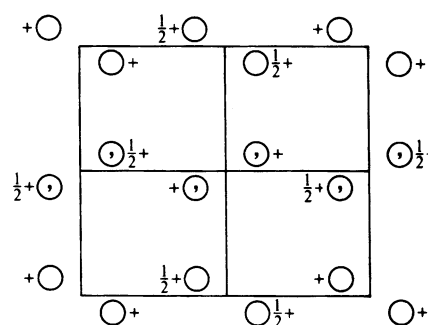
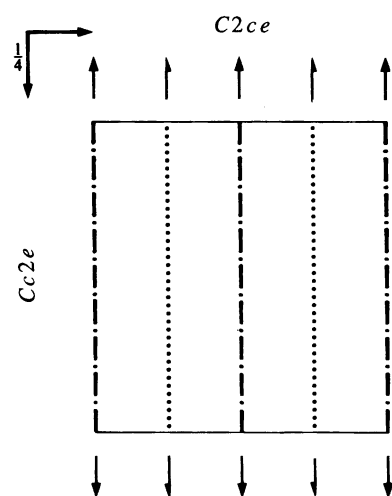
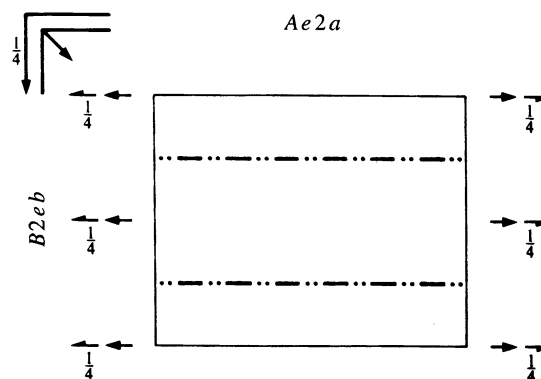
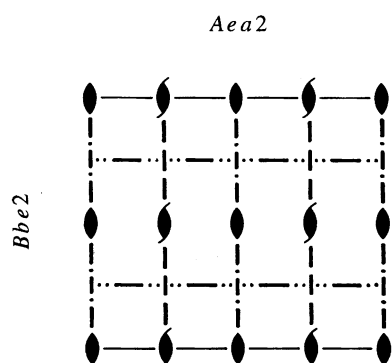
Orthorhombic

No. 41

Aea2

Patterson symmetry *Ammm* (*Cmmm*)

Former space-group symbol *Aba2*; cf. Chapter 1.3



Origin on $1n2$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2 \quad 0,0,z$ (3) $a \quad x, \frac{1}{4}, z$ (4) $b \quad \frac{1}{4}, y, z$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) $t(0, \frac{1}{2}, \frac{1}{2})$ (2) $2(0,0, \frac{1}{2}) \quad 0, \frac{1}{4}, z$ (3) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, 0, z$ (4) $c \quad \frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+			General:

8	<i>b</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(4) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	
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$hkl : k + l = 2n$
 $0kl : k, l = 2n$
 $h0l : h, l = 2n$
 $hk0 : k = 2n$
 $h00 : h = 2n$
 $0k0 : k = 2n$
 $00l : l = 2n$

4	<i>a</i>	..2	0,0, z	$\frac{1}{2}, \frac{1}{2}, z$			
---	----------	-----	----------	-------------------------------	--	--	--

Special: as above, plus

$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p2mg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0, z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $A1a1$ (Cc , 9)	(1; 3)+
	[2] $Ae11$ (Pc , 7)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pbn2_1$ ($Pna2_1$, 33)	1; 4; (2; 3) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $Pba2$ (32)	1; 2; 3; 4
	[2] $Pcn2$ ($Pnc2$, 30)	1; 2; (3; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] $Pca2_1$ (29)	1; 3; (2; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Aea2$ ($\mathbf{a}' = 3\mathbf{a}$) (41); [3] $Aea2$ ($\mathbf{b}' = 3\mathbf{b}$) (41); [3] $Aea2$ ($\mathbf{c}' = 3\mathbf{c}$) (41)

Minimal non-isomorphic supergroups

I [2] $Cmce$ (64); [2] $Ccce$ (68)

II [2] $Fmm2$ (42); [2] $Pma2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (28); [2] $Aem2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (39)

$F m m 2$

C_{2v}^{18}

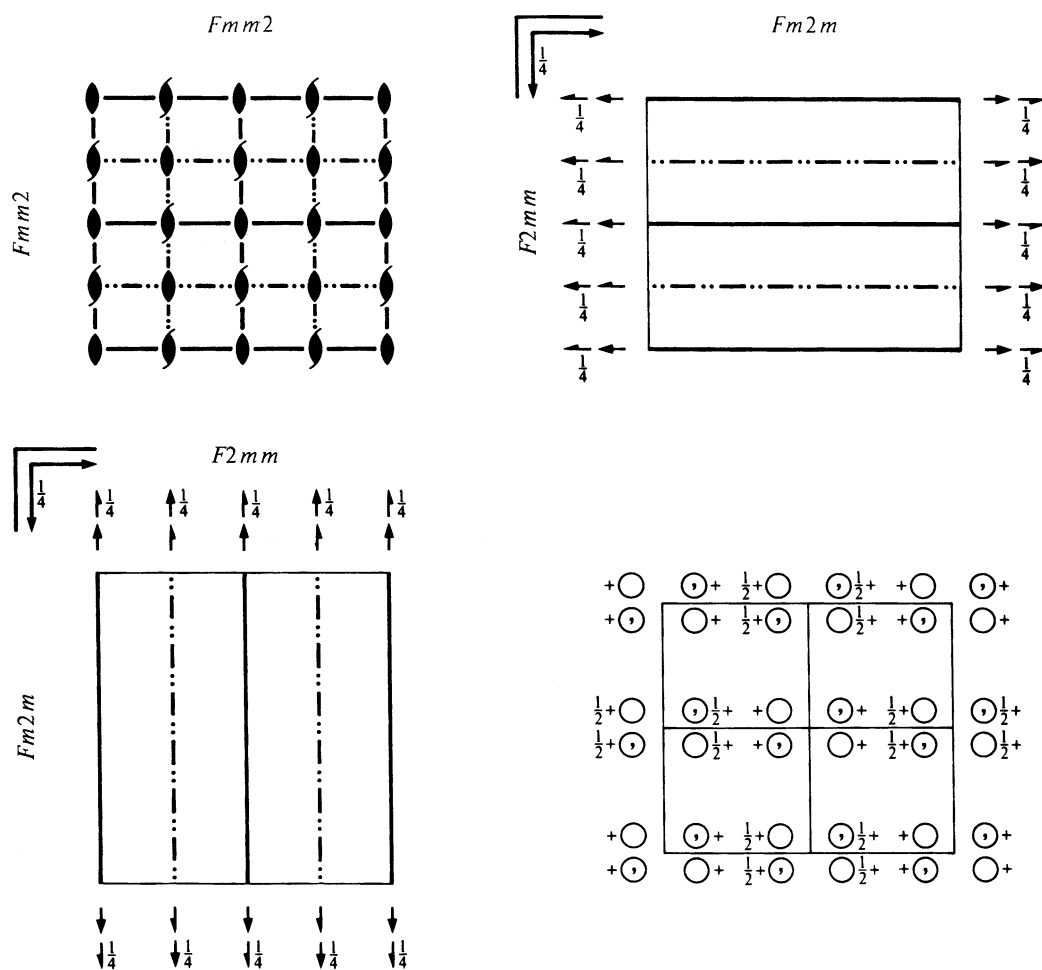
$m m 2$

Orthorhombic

No. 42

$F m m 2$

Patterson symmetry $F m m m$



Origin on $m m 2$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0, 0, 0)+$ set

- (1) 1 (2) $2 \ 0, 0, z$ (3) $m \ x, 0, z$ (4) $m \ 0, y, z$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- (1) $t(0, \frac{1}{2}, \frac{1}{2})$ (2) $2(0, 0, \frac{1}{2}) \ 0, \frac{1}{4}, z$ (3) $c \ x, \frac{1}{4}, z$ (4) $n(0, \frac{1}{2}, \frac{1}{2}) \ 0, y, z$

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ (2) $2(0, 0, \frac{1}{2}) \ \frac{1}{4}, 0, z$ (3) $n(\frac{1}{2}, 0, \frac{1}{2}) \ x, 0, z$ (4) $c \ \frac{1}{4}, y, z$

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ (2) $2 \ \frac{1}{4}, \frac{1}{4}, z$ (3) $a \ x, \frac{1}{4}, z$ (4) $b \ \frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	General:
16 <i>e</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) x,\bar{y},z	(4) \bar{x},y,z	$hkl : h+k, h+l, k+l = 2n$ $Ok l : k, l = 2n$ $hOl : h, l = 2n$ $hk0 : h, k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
8 <i>d</i> . <i>m</i> .	$x,0,z$	$\bar{x},0,z$			Special: as above, plus no extra conditions
8 <i>c</i> <i>m</i> ..	$0,y,z$	$0,\bar{y},z$			no extra conditions
8 <i>b</i> ..2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{3}{4}, z$			$hkl : h = 2n$
4 <i>a</i> <i>m m</i> 2	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] *p2mm*
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [100] *p1m1*
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at x,0,0

Along [010] *p11m*
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] <i>F1m1</i> (<i>Cm</i> , 8)	(1; 3)+
	[2] <i>Fm11</i> (<i>Cm</i> , 8)	(1; 4)+
	[2] <i>F112</i> (<i>C2</i> , 5)	(1; 2)+
IIa	[2] <i>Aea2</i> (41)	1; 2; (1; 2) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] <i>Bbe2</i> (<i>Aea2</i> , 41)	1; 2; (1; 2) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] <i>Ama2</i> (40)	1; 4; (1; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] <i>Bbm2</i> (<i>Ama2</i> , 40)	1; 3; (1; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] <i>Bme2</i> (<i>Aem2</i> , 39)	1; 4; (1; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] <i>Aem2</i> (39)	1; 3; (1; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] <i>Amm2</i> (38)	1; 2; 3; 4; (1; 2; 3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Bmm2</i> (<i>Amm2</i> , 38)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] <i>Ccc2</i> (37)	1; 2; (1; 2) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] <i>Ccm2</i> ₁ (<i>Cmc2</i> ₁ , 36)	1; 3; (1; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] <i>Cmc2</i> ₁ (36)	1; 4; (1; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$
	[2] <i>Cmm2</i> (35)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] *Fmm2* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (42); [3] *Fmm2* ($\mathbf{c}' = 3\mathbf{c}$) (42)

Minimal non-isomorphic supergroups

I [2] *Fmmm* (69); [2] *I4mm* (107); [2] *I4cm* (108); [2] *I42m* (121)

II [2] *Pmm2* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (25)

$Fdd2$

C_{2v}^{19}

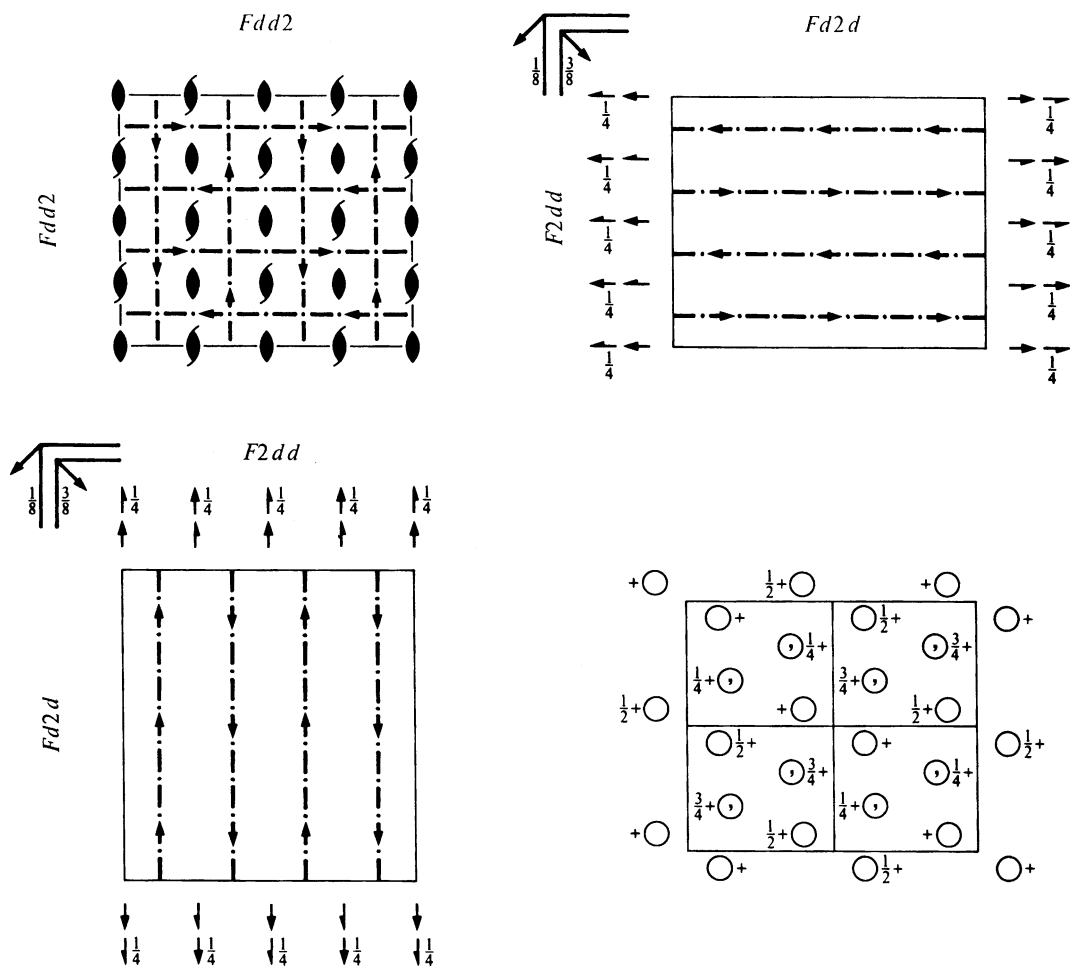
$mm2$

Orthorhombic

No. 43

$Fdd2$

Patterson symmetry $Fmmm$



Origin on 112

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2 \ 0,0,z$ (3) $d(\frac{1}{4},0,\frac{1}{4}) \ x,\frac{1}{8},z$ (4) $d(0,\frac{1}{4},\frac{1}{4}) \ \frac{1}{8},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

- (1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2}) \ 0,\frac{1}{4},z$ (3) $d(\frac{1}{4},0,\frac{3}{4}) \ x,\frac{3}{8},z$ (4) $d(0,\frac{3}{4},\frac{3}{4}) \ \frac{1}{8},y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

- (1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2}) \ \frac{1}{4},0,z$ (3) $d(\frac{3}{4},0,\frac{3}{4}) \ x,\frac{1}{8},z$ (4) $d(0,\frac{1}{4},\frac{3}{4}) \ \frac{3}{8},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2 \ \frac{1}{4},\frac{1}{4},z$ (3) $d(\frac{3}{4},0,\frac{1}{4}) \ x,\frac{3}{8},z$ (4) $d(0,\frac{3}{4},\frac{1}{4}) \ \frac{3}{8},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

(0,0,0)+ (0, $\frac{1}{2}$, $\frac{1}{2}$)+ ($\frac{1}{2}$, 0, $\frac{1}{2}$)+ ($\frac{1}{2}$, $\frac{1}{2}$, 0)+
 16 *b* 1 (1) x, y, z (2) \bar{x}, \bar{y}, z (3) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{1}{4}$ (4) $\bar{x} + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$

General:

hkl : $h+k, h+l, k+l = 2n$
 $0kl$: $k+l = 4n, k, l = 2n$
 $h0l$: $h+l = 4n, h, l = 2n$
 $hk0$: $h, k = 2n$
 $h00$: $h = 4n$
 $0k0$: $k = 4n$
 $00l$: $l = 4n$

Special: as above, plus

hkl : $h = 2n + 1$
 or $h+k+l = 4n$

8 *a* .. 2 0,0,z $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{4}$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [100] $c1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $c11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $F1d1(Cc, 9)$ (1; 3)+
 [2] $Fd11(Cc, 9)$ (1; 4)+
 [2] $F112(C2, 5)$ (1; 2)+

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $Fdd2(\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b})$ (43); [3] $Fdd2(\mathbf{c}' = 3\mathbf{c})$ (43)**Minimal non-isomorphic supergroups****I** [2] $Fddd(70)$; [2] $I4_1md(109)$; [2] $I4_1cd(110)$; [2] $I\bar{4}2d(122)$ **II** [2] $Pnn2(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})$ (34)

*Imm*2

C_{2v}^{20}

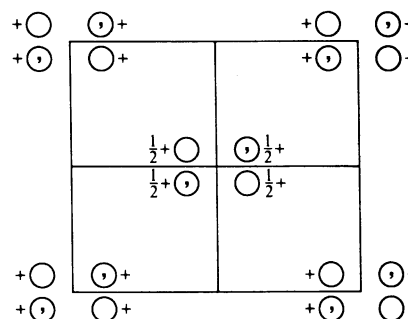
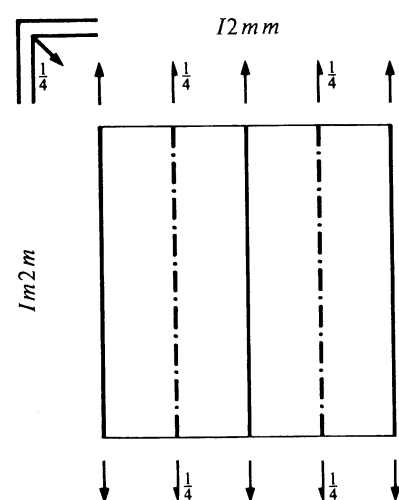
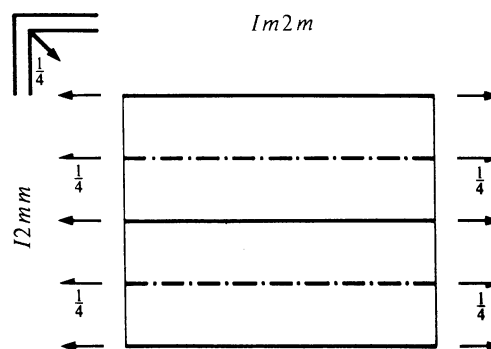
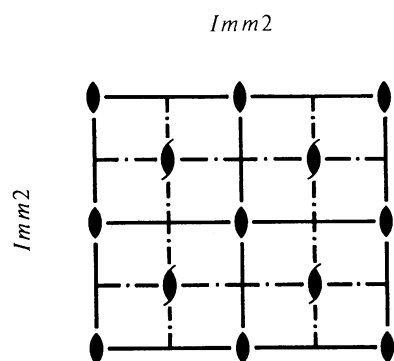
*mm*2

Orthorhombic

No. 44

*Imm*2

Patterson symmetry *Immm*



Origin on *mm*2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- (1) 1 (2) $2 \quad 0,0,z$ (3) $m \quad x,0,z$ (4) $m \quad 0,y,z$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$ (3) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{4}, z$ (4) $n(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

(0,0,0)+ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

8 *e* 1 (1) x,y,z (2) \bar{x},\bar{y},z (3) x,\bar{y},z (4) \bar{x},y,z

General:

$hkl : h+k+l = 2n$
 $0kl : k+l = 2n$
 $h0l : h+l = 2n$
 $hk0 : h+k = 2n$
 $h00 : h = 2n$
 $0k0 : k = 2n$
 $00l : l = 2n$

Special: no extra conditions

4 *d* *m* . . 0, y,z 0, \bar{y},z

4 *c* . *m* . $x,0,z$ $\bar{x},0,z$

2 *b* *m m* 2 0, $\frac{1}{2},z$

2 *a* *m m* 2 0,0, z

Symmetry of special projectionsAlong [001] *c 2 m m* $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0,0, z Along [100] *c 1 m 1* $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$ Along [010] *c 1 1 m* $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0, $y,0$ **Maximal non-isomorphic subgroups**

I [2] *I 1 m 1* (*Cm*, 8) (1; 3)+
 [2] *I m 1 1* (*Cm*, 8) (1; 4)+
 [2] *I 1 1 2* (*C2*, 5) (1; 2)+

IIa [2] *P n n 2* (34) 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] *P n m 2*₁ (*P m n 2*₁, 31) 1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] *P m n 2*₁ (31) 1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] *P m m 2* (25) 1; 2; 3; 4

IIb none**Maximal isomorphic subgroups of lowest index****IIc** [3] *Imm2* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (44); [3] *Imm2* ($\mathbf{c}' = 3\mathbf{c}$) (44)**Minimal non-isomorphic supergroups****I** [2] *Immm* (71); [2] *Imma* (74); [2] *I4mm* (107); [2] *I4,md* (109); [2] *I4m2* (119)**II** [2] *Cmm2* ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (35); [2] *Amm2* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (38); [2] *Bmm2* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (*Amm2*, 38)

*Iba*2

C_{2v}^{21}

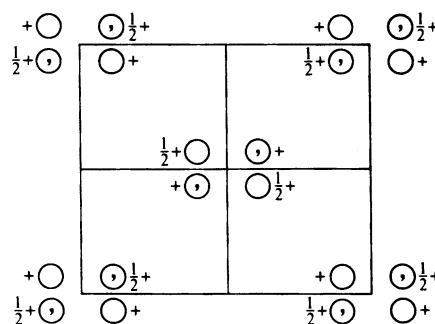
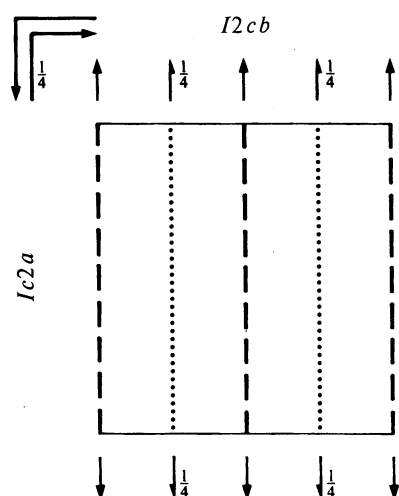
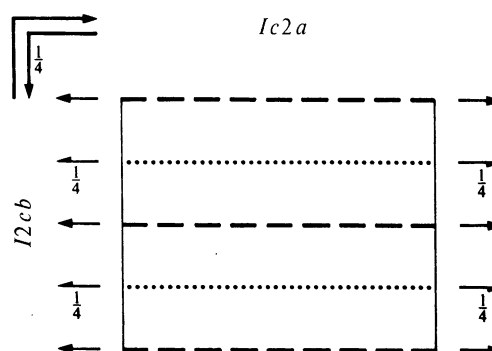
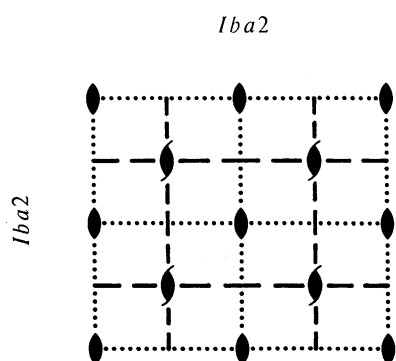
*mm*2

Orthorhombic

No. 45

*Iba*2

Patterson symmetry *Immm*



Origin on *cc*2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- (1) 1 (2) 2 $0,0,z$ (3) *a* $x, \frac{1}{4}, z$ (4) *b* $\frac{1}{4}, y, z$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

- (1) *t* $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) 2 $(0,0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ (3) *c* $x, 0, z$ (4) *c* $0, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8 c 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$hkl : h+k+l=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
4 b ..2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			Special: as above, plus $hkl : l=2n$
4 a ..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			$hkl : l=2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0,0,z

Along [100] $p1m1$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,0,0

Along [010] $p11m$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $I1a1 (Cc, 9)$	(1; 3)+
	[2] $Ib11 (Cc, 9)$	(1; 4)+
	[2] $I112 (C2, 5)$	(1; 2)+
IIa	[2] $Pba2 (32)$	1; 2; 3; 4
	[2] $Pca2_1 (29)$	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbc2_1 (Pca2_1, 29)$	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcc2 (27)$	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Iba2 (\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}) (45)$; [3] $Iba2 (\mathbf{c}' = 3\mathbf{c}) (45)$

Minimal non-isomorphic supergroups

I [2] $Ibam (72)$; [2] $Ibca (73)$; [2] $I4cm (108)$; [2] $I4_1cd (110)$; [2] $I\bar{4}c2 (120)$
II [2] $Cmm2 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (35)$; [2] $Aem2 (\mathbf{a}' = \frac{1}{2}\mathbf{a}) (39)$; [2] $Bme2 (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (Aem2, 39)$

Ima2

C_{2v}^{22}

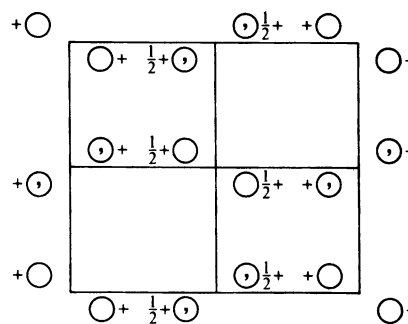
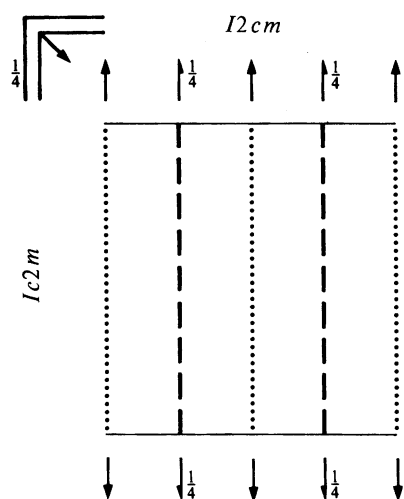
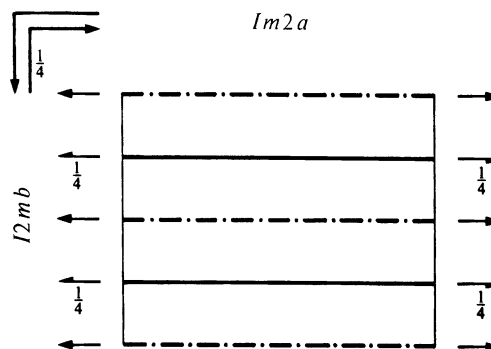
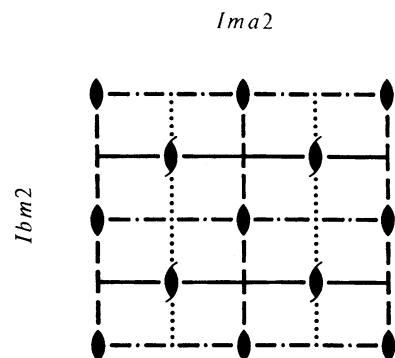
mm2

Orthorhombic

No. 46

Ima2

Patterson symmetry *Immm*



Origin on *na2*

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) $2 \quad 0,0,z$ (3) $a \quad x,0,z$ (4) $m \quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$ (3) $c \quad x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2}) \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
8 <i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	$hkl : h+k+l=2n$ $0kl : k+l=2n$ $h0l : h,l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
4 <i>b</i> <i>m</i> . .	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			Special: as above, plus no extra conditions
4 <i>a</i> . . 2	$0,0,z$	$\frac{1}{2},0,z$			$hkl : h=2n$

Symmetry of special projections

Along [001] *c2mm*

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] *c1m1*

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [010] *p11m*

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] <i>I1a1</i> (<i>Cc</i> , 9)	(1; 3)+
	[2] <i>Im11</i> (<i>Cm</i> , 8)	(1; 4)+
	[2] <i>I112</i> (<i>C2</i> , 5)	(1; 2)+
IIa	[2] <i>Pna2</i> ₁ (33)	1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pnc2</i> (30)	1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pma2</i> (28)	1; 2; 3; 4
	[2] <i>Pmc2</i> ₁ (26)	1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] *Ima2* ($\mathbf{a}' = 3\mathbf{a}$) (46); [3] *Ima2* ($\mathbf{b}' = 3\mathbf{b}$) (46); [3] *Ima2* ($\mathbf{c}' = 3\mathbf{c}$) (46)

Minimal non-isomorphic supergroups

I	[2] <i>Ibam</i> (72); [2] <i>Imma</i> (74)
II	[2] <i>Cmm2</i> ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (35); [2] <i>Amm2</i> ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (38); [2] <i>Bme2</i> ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (<i>Aem2</i> , 39)

$Pmmm$

D_{2h}^1

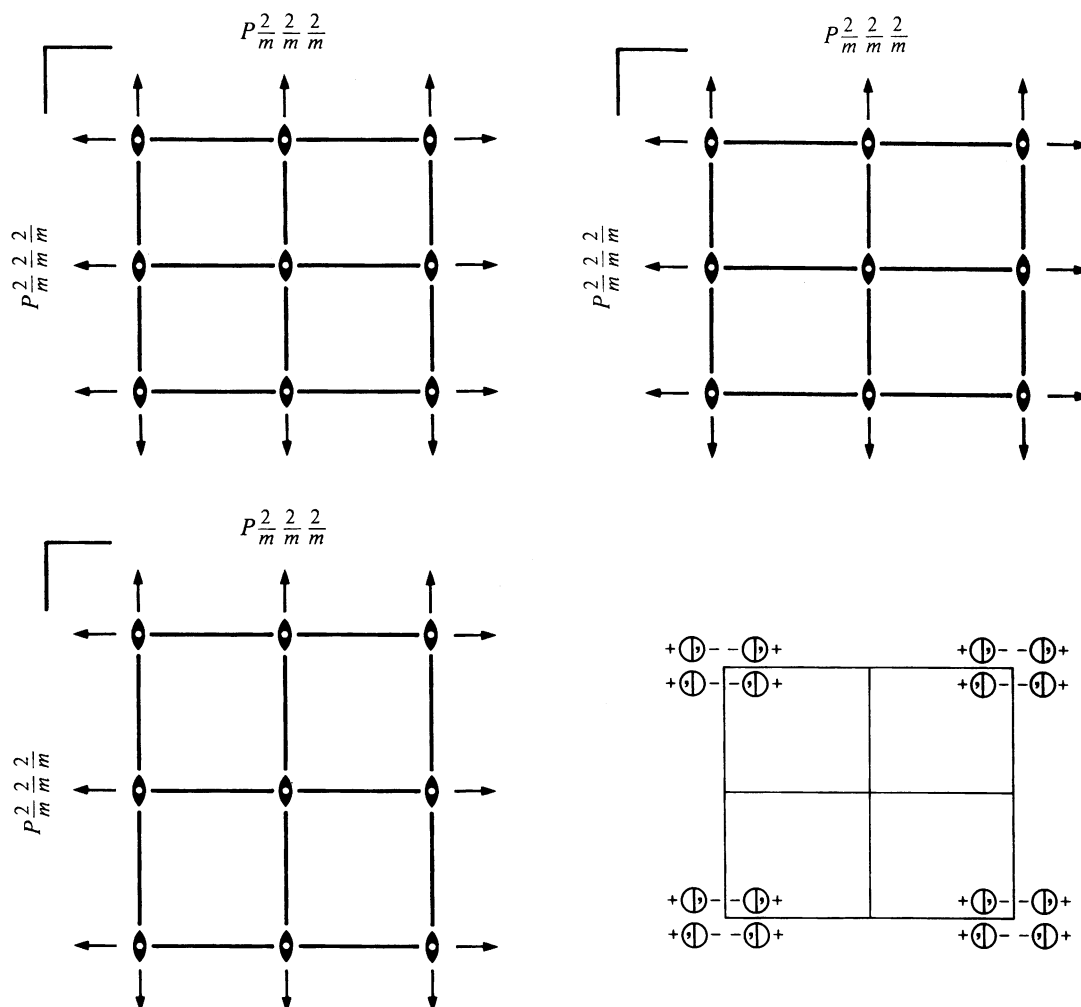
mmm

Orthorhombic

No. 47

$P 2/m 2/m 2/m$

Patterson symmetry $Pmmm$



Origin at centre (mmm)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------|-----------------|-----------------|-----------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) m $x,y,0$ | (7) m $x,0,z$ | (8) m $0,y,z$ |

Maximal non-isomorphic subgroups (*continued*)

IIa none

IIb [2] $Pmma$ ($\mathbf{a}' = 2\mathbf{a}$) (51); [2] $Pmam$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pmma$, 51); [2] $Pmaa$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pccm$, 49); [2] $Pbmm$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmma$, 51); [2] $Pmmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmma$, 51); [2] $Pbmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pccm$, 49); [2] $Pcmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmma$, 51); [2] $Pmcm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmma$, 51); [2] $Pccm$ ($\mathbf{c}' = 2\mathbf{c}$) (49); [2] $Aemm$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmme$, 67); [2] $Ammm$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmmm$, 65); [2] $Bmem$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cmme$, 67); [2] $Bmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cmmm$, 65); [2] $Cmme$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (67); [2] $Cmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (65); [2] $Fmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (69)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmmm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$) (47)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4_2/mmc$ (131); [3] $Pm\bar{3}$ (200)

II [2] $Ammm$ ($Cmmm$, 65); [2] $Bmmm$ ($Cmmm$, 65); [2] $Cmmm$ (65); [2] $Immm$ (71)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions	
						General:	
8	α 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) \bar{x}, y, \bar{z} (7) x, \bar{y}, z	(4) x, \bar{y}, \bar{z} (8) \bar{x}, y, z	no conditions	
Special: no extra conditions							
4	z . . m	$x, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$	$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$		
4	y . . m	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, 0$	$x, \bar{y}, 0$		
4	x . m .	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, \bar{z}$	$x, \frac{1}{2}, \bar{z}$		
4	w . m .	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x}, 0, \bar{z}$	$x, 0, \bar{z}$		
4	v m . .	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$	$\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, \bar{z}$		
4	u m . .	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$		
2	t $m m 2$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$				
2	s $m m 2$	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$				
2	r $m m 2$	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$				
2	q $m m 2$	$0, 0, z$	$0, 0, \bar{z}$				
2	p $m 2 m$	$\frac{1}{2}, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	1	h $m m m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
2	o $m 2 m$	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	1	g $m m m$	$0, \frac{1}{2}, \frac{1}{2}$	
2	n $m 2 m$	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$	1	f $m m m$	$\frac{1}{2}, \frac{1}{2}, 0$	
2	m $m 2 m$	$0, y, 0$	$0, \bar{y}, 0$	1	e $m m m$	$0, \frac{1}{2}, 0$	
2	l $2 m m$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	1	d $m m m$	$\frac{1}{2}, 0, \frac{1}{2}$	
2	k $2 m m$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	1	c $m m m$	$0, 0, \frac{1}{2}$	
2	j $2 m m$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	1	b $m m m$	$\frac{1}{2}, 0, 0$	
2	i $2 m m$	$x, 0, 0$	$\bar{x}, 0, 0$	1	a $m m m$	$0, 0, 0$	

Symmetry of special projections

Along $[001]$ $p2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[010]$ $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pmm2$ (25)	1; 2; 7; 8
	[2] $Pm2m$ ($Pmm2$, 25)	1; 3; 6; 8
	[2] $P2mm$ ($Pmm2$, 25)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 5; 6
	[2] $P12/m1$ ($P2/m$, 10)	1; 3; 5; 7
	[2] $P2/m11$ ($P2/m$, 10)	1; 4; 5; 8

(Continued on preceding page)

$Pn\bar{1}n$

D_{2h}^2

mmm

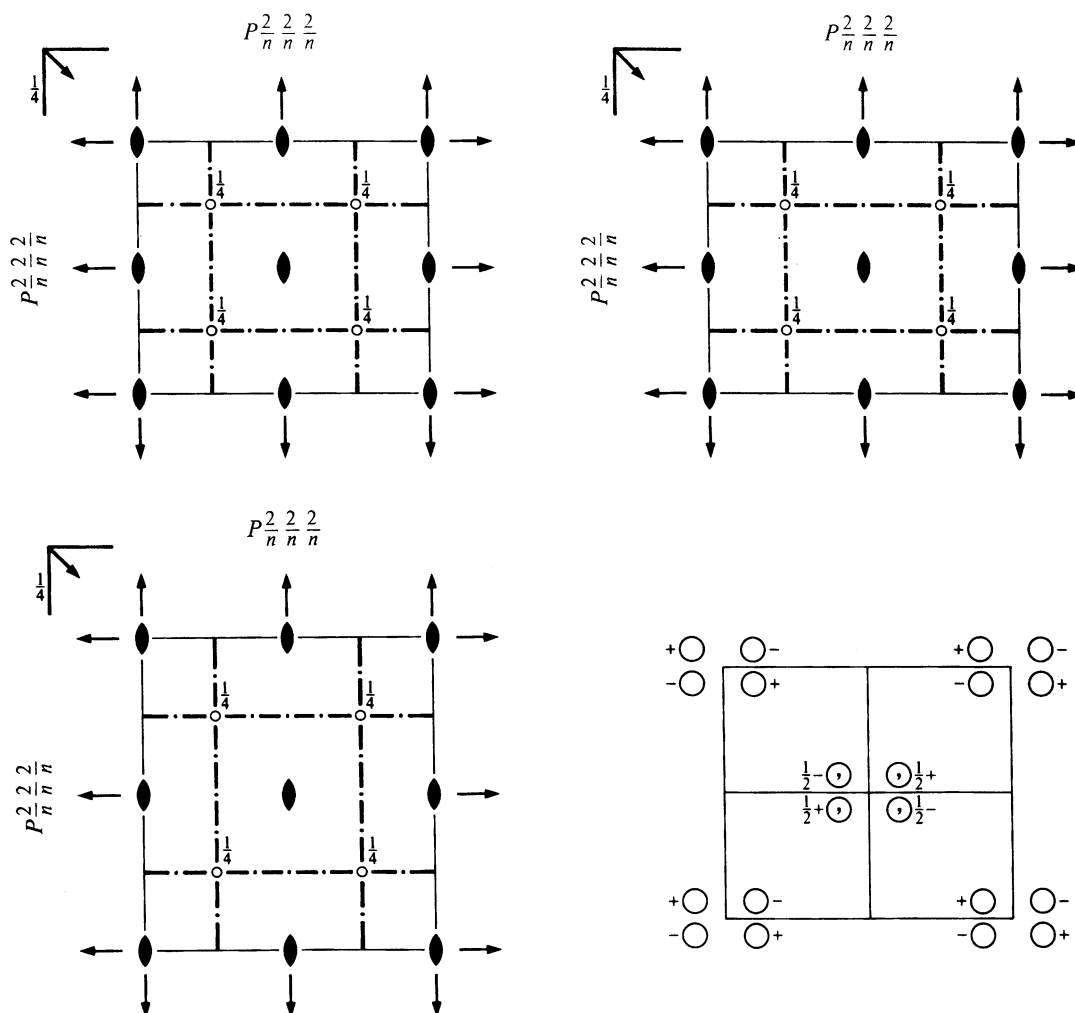
Orthorhombic

No. 48

$P 2/n 2/n 2/n$

Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at 222 , at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- | | | | |
|---|--|--|--|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |

Minimal non-isomorphic supergroups

- I** [2] $P4/nnc$ (126); [2] $P4_2/nnm$ (134); [3] $Pn\bar{3}$ (201)
- II** [2] $Immm$ (71); [2] $Amaa$ ($Cccm$, 66); [2] $Bbmb$ ($Cccm$, 66); [2] $Cccm$ (66); [2] $Pncb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pban$, 50); [2] $Pcna$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pban$, 50); [2] $Pban$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (50)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry						General:
8	<i>m</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) \bar{x}, y, \bar{z} (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) x, \bar{y}, \bar{z} (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	$Ok\bar{l} : k + l = 2n$ $h0\bar{l} : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00\bar{l} : l = 2n$
						Special: as above, plus
4	<i>l</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>k</i> ..2	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>j</i> .2.	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	$0, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, y + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>i</i> .2.	$0, y, 0$	$0, \bar{y}, 0$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>h</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$x + \frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
4	<i>g</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>f</i> $\bar{1}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4	<i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
2	<i>d</i> 222	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	<i>c</i> 222	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2	<i>b</i> 222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	<i>a</i> 222	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $c2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at x, 0, 0

Along [010] $c2mm$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at 0, y, 0

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2n$ ($Pnn2$, 34)	1; 3; 6; 8
	[2] $P2nn$ ($Pnn2$, 34)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/n11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb [2] $Fddd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (70)

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnnn$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (48)

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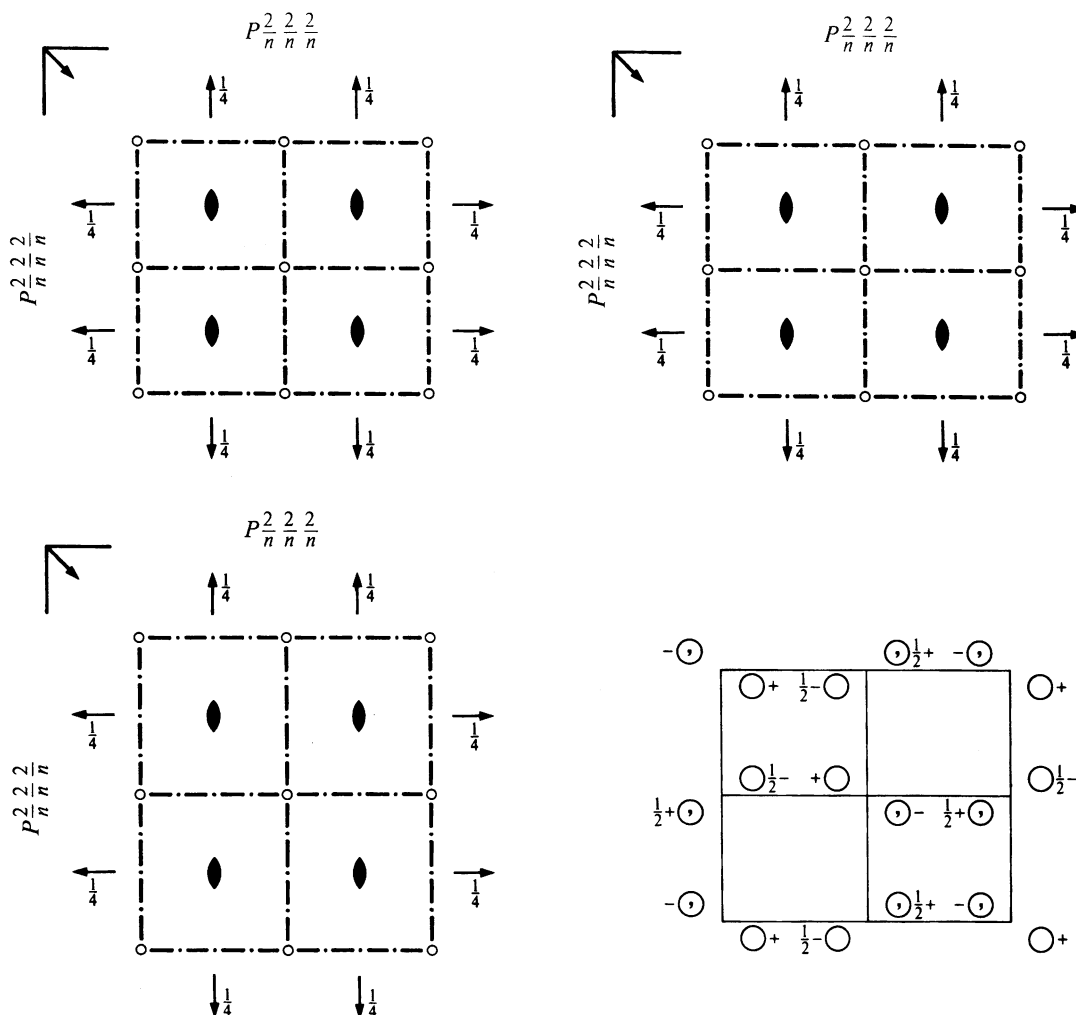
$Pn\bar{1}$ D_{2h}^2 mmm

Orthorhombic

No. 48

 $P 2_1/n 2_1/n 2_1/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at nnn , at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from 222Asymmetric unit $0 \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- | | | | |
|---------------------|--|--|--|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2 $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1}$ 0,0,0 | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ |

Maximal isomorphic subgroups of lowest index

IIc [3] $Pn\bar{1}$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (48)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4_2/nm$ (134); [3] $Pn\bar{3}$ (201)II [2] $Immm$ (71); [2] $Amaa$ ($Cccm$, 66); [2] $Bbmb$ ($Cccm$, 66); [2] $Cccm$ (66); [2] $Pncb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pban$, 50); [2] $Pcna$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pban$, 50); [2] $Pban$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (50)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>m</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	General: $Ok\bar{l} : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : h + k + l = 2n$
4 <i>l</i> ..2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>k</i> ..2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>j</i> .2.	$\frac{3}{4}, y, \frac{1}{4}$	$\frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4 <i>i</i> .2.	$\frac{1}{4}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \frac{3}{4}$	$\frac{3}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4 <i>h</i> 2..	$x, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
4 <i>g</i> 2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4 <i>f</i> $\bar{1}$	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>e</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, $\frac{1}{2}$	0, $\frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
2 <i>d</i> 222	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$
2 <i>c</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$			$hkl : h + k + l = 2n$
2 <i>b</i> 222	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$
2 <i>a</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $c2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [010] $c2mm$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $\frac{1}{4}, y, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2n$ ($Pnn2$, 34)	1; 3; 6; 8
	[2] $P2nn$ ($Pnn2$, 34)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/n11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb [2] $Fddd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (70)

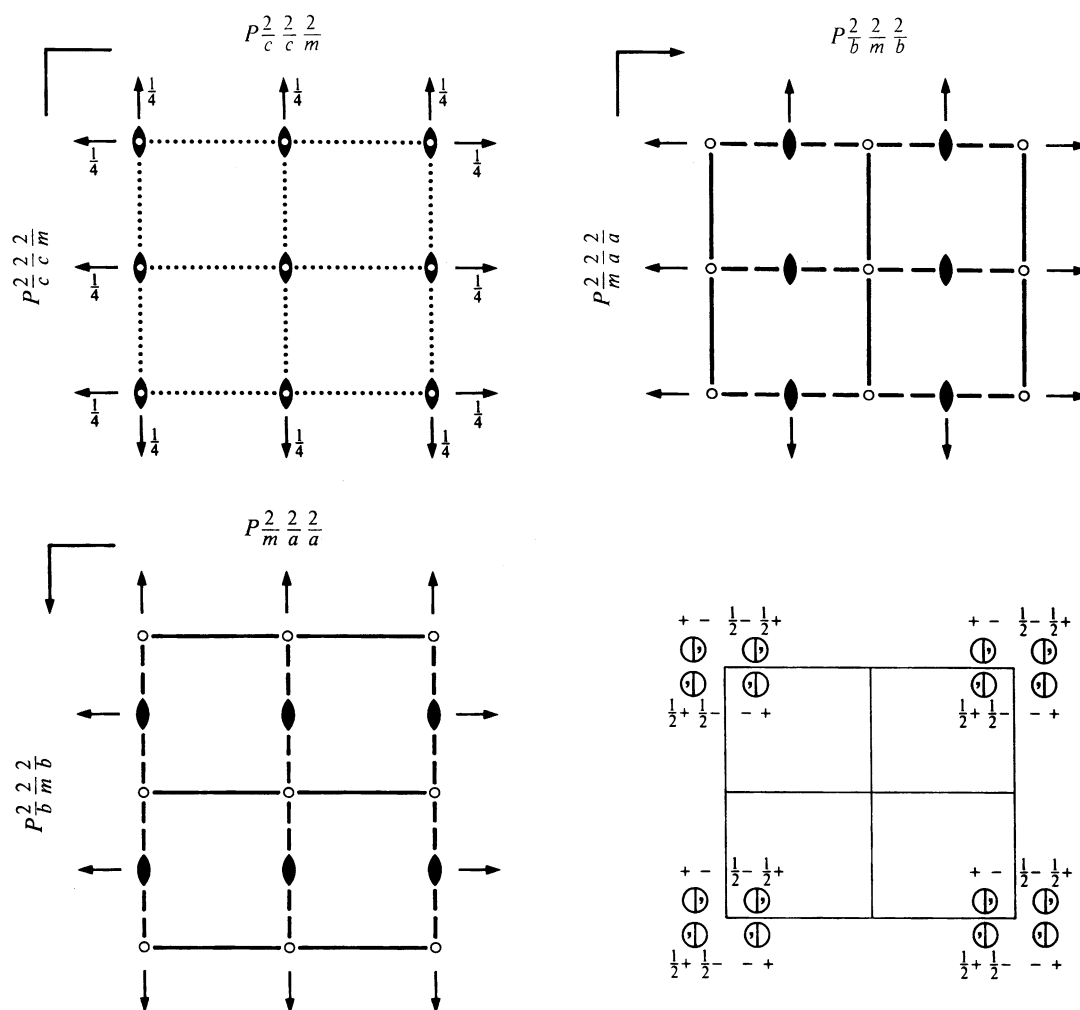
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$Pccm$
 D_{2h}^3
 mmm

Orthorhombic

No. 49

 $P 2/c 2/c 2/m$

 Patterson symmetry $Pmmm$

 Origin at centre ($2/m$) at $cc2/m$

 Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------|-------------------|---------------------------|---------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, \frac{1}{4}$ | (4) 2 $x, 0, \frac{1}{4}$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) m $x, y, 0$ | (7) c $x, 0, z$ | (8) c $0, y, z$ |

Maximal non-isomorphic subgroups (continued)

IIa none

IIb $[2] Pcca$ ($\mathbf{a}' = 2\mathbf{a}$) (54); $[2] Pcnm$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pmna$, 53); $[2] Pcna$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pban$, 50); $[2] Pccb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pcca$, 54);
 $[2] Pncm$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmna$, 53); $[2] Pncb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pban$, 50); $[2] Ccce$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (68); $[2] Cccm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (66)

Maximal isomorphic subgroups of lowest index

IIc $[2] Pccm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (49); $[3] Pccm$ ($\mathbf{c}' = 3\mathbf{c}$) (49)

Minimal non-isomorphic supergroups

I $[2] P4/mcc$ (124); $[2] P4_2/mcm$ (132)

II $[2] Cccm$ (66); $[2] Aemm$ ($Cmme$, 67); $[2] Bmem$ ($Cmme$, 67); $[2] Ibam$ (72); $[2] Pmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (47)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	<i>r</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y}, z + \frac{1}{2}$	(4) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y, z + \frac{1}{2}$	$Ok\bar{l} : l = 2n$ $h0l : l = 2n$ $00l : l = 2n$
						Special: as above, plus
4	<i>q</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$	no extra conditions
4	<i>p</i> .. 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4	<i>o</i> .. 2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4	<i>n</i> .. 2	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4	<i>m</i> .. 2	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4	<i>l</i> . 2 .	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$	$\frac{1}{2}, y, \frac{3}{4}$	$hkl : l = 2n$
4	<i>k</i> . 2 .	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$	$0, y, \frac{3}{4}$	$hkl : l = 2n$
4	<i>j</i> 2 ..	$x, \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \frac{1}{2}, \frac{3}{4}$	$x, \frac{1}{2}, \frac{3}{4}$	$hkl : l = 2n$
4	<i>i</i> 2 ..	$x, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$x, 0, \frac{3}{4}$	$hkl : l = 2n$
2	<i>h</i> 2 2 2	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2	<i>g</i> 2 2 2	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2	<i>f</i> 2 2 2	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$			$hkl : l = 2n$
2	<i>e</i> 2 2 2	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$
2	<i>d</i> .. 2/ <i>m</i>	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : l = 2n$
2	<i>c</i> .. 2/ <i>m</i>	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	<i>b</i> .. 2/ <i>m</i>	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	<i>a</i> .. 2/ <i>m</i>	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [010] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pc2m$ ($Pma2$, 28)	1; 3; 6; 8
	[2] $P2cm$ ($Pma2$, 28)	1; 4; 6; 7
	[2] $Pcc2$ (27)	1; 2; 7; 8
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/c11$ ($P2/c$, 13)	1; 4; 5; 8
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 5; 6

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Pban

D_{2h}^4

mmm

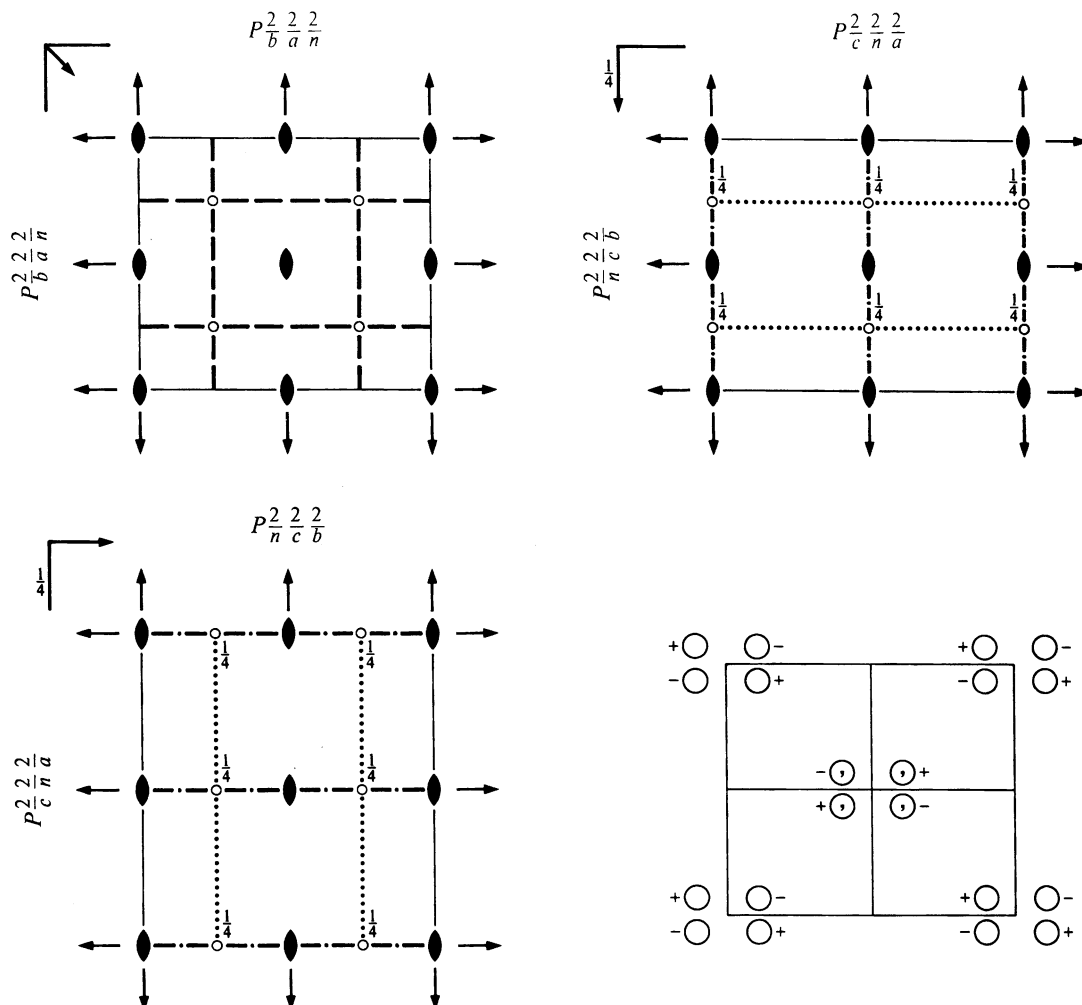
Orthorhombic

No. 50

$P\ 2/b\ 2/a\ 2/n$

Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $222/n$, at $\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---|--|-----------------------------|-----------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (7) a $x, \frac{1}{4}, z$ | (8) b $\frac{1}{4}, y, z$ |

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II [2] $Cmmm$ (65); [2] $Aeaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>m</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	General: $Ok\bar{l} : k = 2n$ $h0l : h = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$
	(5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	
4 <i>l</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, 0, z$	$hkl : h + k = 2n$
4 <i>k</i> ..2	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hkl : h + k = 2n$
4 <i>j</i> .2.	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
4 <i>i</i> .2.	$0, y, 0$	$0, \bar{y}, 0$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	$\frac{1}{2}, y + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 <i>h</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
4 <i>g</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$x + \frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 <i>f</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h, k = 2n$
2 <i>d</i> 222	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>c</i> 222	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>b</i> 222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$			$hkl : h + k = 2n$
2 <i>a</i> 222	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, 0, 0

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0, y, 0

Maximal non-isomorphic subgroups

I [2] $Pba2$ (32) 1; 2; 7; 8
 [2] $Pb2n$ ($Pnc2$, 30) 1; 3; 6; 8
 [2] $P2an$ ($Pnc2$, 30) 1; 4; 6; 7
 [2] $P222$ (16) 1; 2; 3; 4
 [2] $P112/n$ ($P2/c$, 13) 1; 2; 5; 6
 [2] $P12/a1$ ($P2/c$, 13) 1; 3; 5; 7
 [2] $P2/b11$ ($P2/c$, 13) 1; 4; 5; 8

IIa none

IIb [2] $Pnan$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}' = 2\mathbf{c}$) (48)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pban$ ($\mathbf{c}' = 2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (50)

(Continued on preceding page)

Pban

D_{2h}^4

mmm

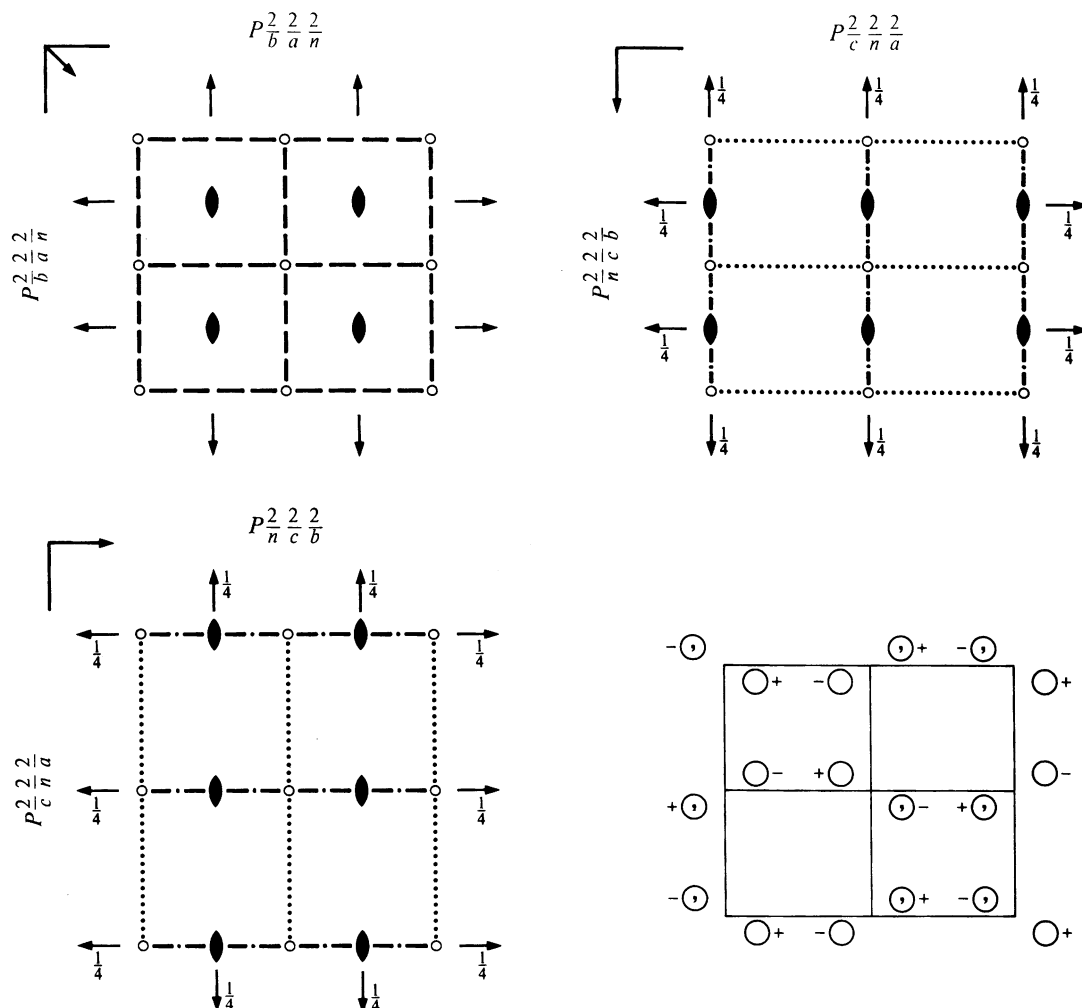
Orthorhombic

No. 50

$P 2/b 2/a 2/n$

Patterson symmetry *Pmmm*

ORIGIN CHOICE 2



Origin at $\bar{1}$ at *ban*, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from 222

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------|--|---------------------------|---------------------------|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $2 \frac{1}{4}, y, 0$ | (4) $2 x, \frac{1}{4}, 0$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (7) $a x, 0, z$ | (8) $b 0, y, z$ |

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II [2] $Cmmm$ (65); [2] $Aaaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>m</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (7) $x + \frac{1}{2}, \bar{y}, z$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x}, y + \frac{1}{2}, z$	General: $Ok\bar{l} : k = 2n$ $h0l : h = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ Special: as above, plus
4 <i>l</i> ..2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, z$	$hkl : h + k = 2n$
4 <i>k</i> ..2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{3}{4}, z$	$hkl : h + k = 2n$
4 <i>j</i> .2.	$\frac{1}{4}, y, \frac{1}{2}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\frac{3}{4}, \bar{y}, \frac{1}{2}$	$\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
4 <i>i</i> .2.	$\frac{1}{4}, y, 0$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, 0$	$\frac{3}{4}, \bar{y}, 0$	$\frac{3}{4}, y + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 <i>h</i> 2..	$x, \frac{1}{4}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}$	$\bar{x}, \frac{3}{4}, \frac{1}{2}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k = 2n$
4 <i>g</i> 2..	$x, \frac{1}{4}, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, 0$	$\bar{x}, \frac{3}{4}, 0$	$x + \frac{1}{2}, \frac{3}{4}, 0$	$hkl : h + k = 2n$
4 <i>f</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>e</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$hkl : h, k = 2n$
2 <i>d</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>c</i> 222	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>b</i> 222	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$			$hkl : h + k = 2n$
2 <i>a</i> 222	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pba2$ (32)	1; 2; 7; 8
	[2] $Pb2n$ ($Pnc2$, 30)	1; 3; 6; 8
	[2] $P2an$ ($Pnc2$, 30)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/a1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/b11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb [2] $Pnan$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}' = 2\mathbf{c}$) (48)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pban$ ($\mathbf{c}' = 2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (50)

(Continued on preceding page)

$Pmma$

D_{2h}^5

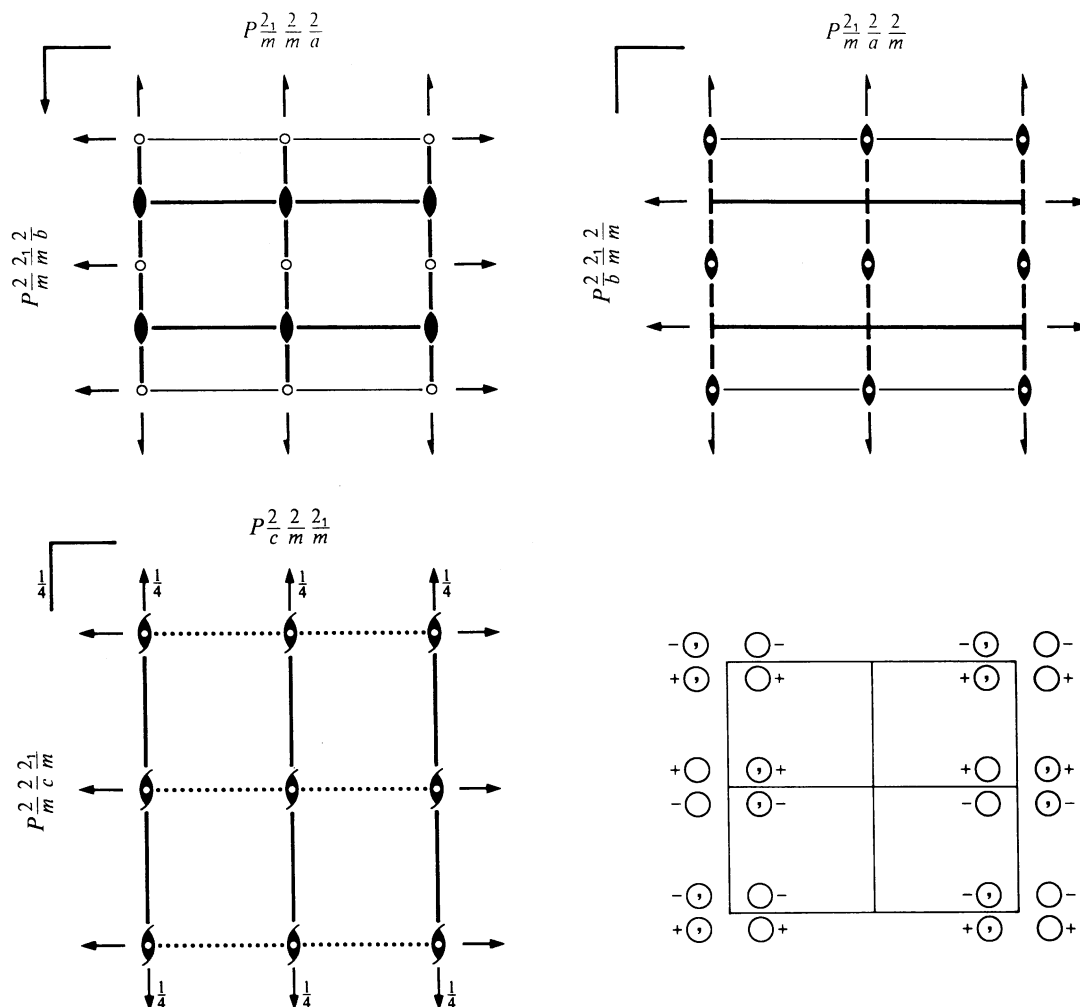
mmm

Orthorhombic

No. 51

$P 2_1/m 2/m 2/a$

Patterson symmetry $Pmmm$



Origin at centre ($2/m$) at $2_1 2/m a$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- | | | | |
|-----------------------|---------------------------|-----------------|------------------------------------|
| (1) 1 | (2) $2 \frac{1}{4}, 0, z$ | (3) $2 0, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) x, 0, 0$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $a x, y, 0$ | (7) $m x, 0, z$ | (8) $m \frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>l</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$ (2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (6) $x + \frac{1}{2}, y, \bar{z}$ (3) \bar{x}, y, \bar{z} (7) x, \bar{y}, z (4) $x + \frac{1}{2}, \bar{y}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y, z$	General: $hk0 : h = 2n$ $h00 : h = 2n$ Special: as above, plus
4 <i>k</i> $m..$	$\frac{1}{4}, y, z$ $\frac{1}{4}, \bar{y}, z$ $\frac{3}{4}, y, \bar{z}$ $\frac{3}{4}, \bar{y}, \bar{z}$	no extra conditions
4 <i>j</i> $.m.$	$x, \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$ $x + \frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
4 <i>i</i> $.m.$	$x, 0, z$ $\bar{x} + \frac{1}{2}, 0, z$ $\bar{x}, 0, \bar{z}$ $x + \frac{1}{2}, 0, \bar{z}$	no extra conditions
4 <i>h</i> $.2.$	$0, y, \frac{1}{2}$ $\frac{1}{2}, \bar{y}, \frac{1}{2}$ $0, \bar{y}, \frac{1}{2}$ $\frac{1}{2}, y, \frac{1}{2}$	$hkl : h = 2n$
4 <i>g</i> $.2.$	$0, y, 0$ $\frac{1}{2}, \bar{y}, 0$ $0, \bar{y}, 0$ $\frac{1}{2}, y, 0$	$hkl : h = 2n$
2 <i>f</i> $mm2$	$\frac{1}{4}, \frac{1}{2}, z$ $\frac{3}{4}, \frac{1}{2}, \bar{z}$	no extra conditions
2 <i>e</i> $mm2$	$\frac{1}{4}, 0, z$ $\frac{3}{4}, 0, \bar{z}$	no extra conditions
2 <i>d</i> $.2/m.$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h = 2n$
2 <i>c</i> $.2/m.$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h = 2n$
2 <i>b</i> $.2/m.$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h = 2n$
2 <i>a</i> $.2/m.$	$0, 0, 0$ $\frac{1}{2}, 0, 0$	$hkl : h = 2n$

Symmetry of special projectionsAlong [001] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along [100] $p2mm$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$ Along [010] $p2gm$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at $0, y, 0$ **Maximal non-isomorphic subgroups**

I	[2] $Pm2a$ ($Pma2$, 28)	1; 3; 6; 8
	[2] $P2_1ma$ ($Pmc2_1$, 26)	1; 4; 6; 7
	[2] $Pmm2$ (25)	1; 2; 7; 8
	[2] $P2_122$ ($P222_1$, 17)	1; 2; 3; 4
	[2] $P112/a$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P2_1/m11$ ($P2_1/m$, 11)	1; 4; 5; 8
	[2] $P12/m1$ ($P2/m$, 10)	1; 3; 5; 7

IIa none

IIb [2] $Pmnm$ ($\mathbf{b}' = 2\mathbf{b}$) (59); [2] $Pbma$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pbcm$, 57); [2] $Pbmn$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmna$, 53); [2] $Pmca$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pbcm$, 57);
[2] $Pcma$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pbam$, 55); [2] $Pcca$ ($\mathbf{c}' = 2\mathbf{c}$) (54); [2] $Aema$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmce$, 64);
[2] $Amma$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmcm$, 63)

Maximal isomorphic subgroups of lowest index**IIc** [2] $Pmma$ ($\mathbf{b}' = 2\mathbf{b}$) (51); [2] $Pmma$ ($\mathbf{c}' = 2\mathbf{c}$) (51); [3] $Pmma$ ($\mathbf{a}' = 3\mathbf{a}$) (51)**Minimal non-isomorphic supergroups****I** none**II** [2] $Amma$ ($Cmcm$, 63); [2] $Bmmm$ ($Cmmm$, 65); [2] $Cmme$ (67); [2] $Imma$ (74); [2] $Pmmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (47)

Pnna

D_{2h}^6

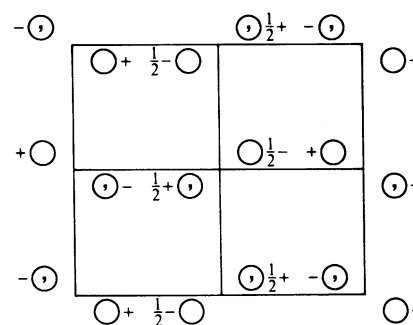
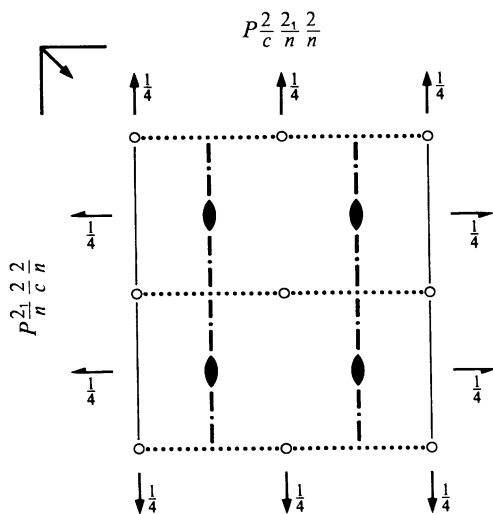
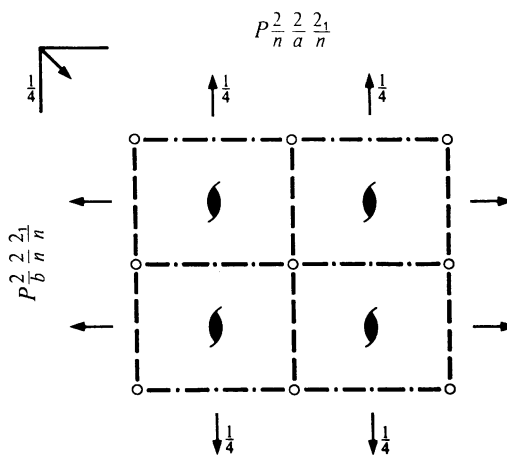
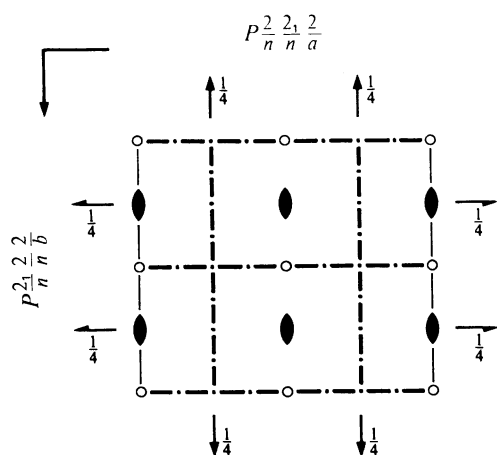
mmm

Orthorhombic

No. 52

$P 2/n 2_1/n 2/a$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $n1a$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------|---------------------------|--|--|
| (1) 1 | (2) $2 \frac{1}{2}, 0, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{1}{4}, y, \frac{1}{4}$ | (4) $2 x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $a x, y, 0$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2}) x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>e</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (6) $x + \frac{1}{2}, y, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	General: $Ok\bar{l} : k + l = 2n$ $h0\bar{l} : h + l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00\bar{l} : l = 2n$ Special: as above, plus
4 <i>d</i> 2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + l = 2n$
4 <i>c</i> ..2	$\frac{1}{4}, 0, z$	$\frac{1}{4}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, 0, \bar{z}$	$\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, 0$	$hkl : h, k + l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k + l = 2n$

Symmetry of special projections

Along [001] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $\frac{1}{4}, y, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2_1a$ ($Pna2_1$, 33)	1; 3; 6; 8
	[2] $P2na$ ($Pnc2$, 30)	1; 4; 6; 7
	[2] $P22_12$ ($P222_1$, 17)	1; 2; 3; 4
	[2] $P12_1/n1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P112/a$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P2/n11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnna$ ($\mathbf{a}' = 3\mathbf{a}$) (52); [3] $Pnna$ ($\mathbf{b}' = 3\mathbf{b}$) (52); [3] $Pnna$ ($\mathbf{c}' = 3\mathbf{c}$) (52)

Minimal non-isomorphic supergroups

I none

II [2] $Bbmm$ ($Cmcm$, 63); [2] $Amaa$ ($Cccm$, 66); [2] $Ccce$ (68); [2] $Imma$ (74); [2] $Pncm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmna$, 53); [2] $Pcna$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pban$, 50); [2] $Pbaa$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pcca$, 54)

$Pmna$

D_{2h}^7

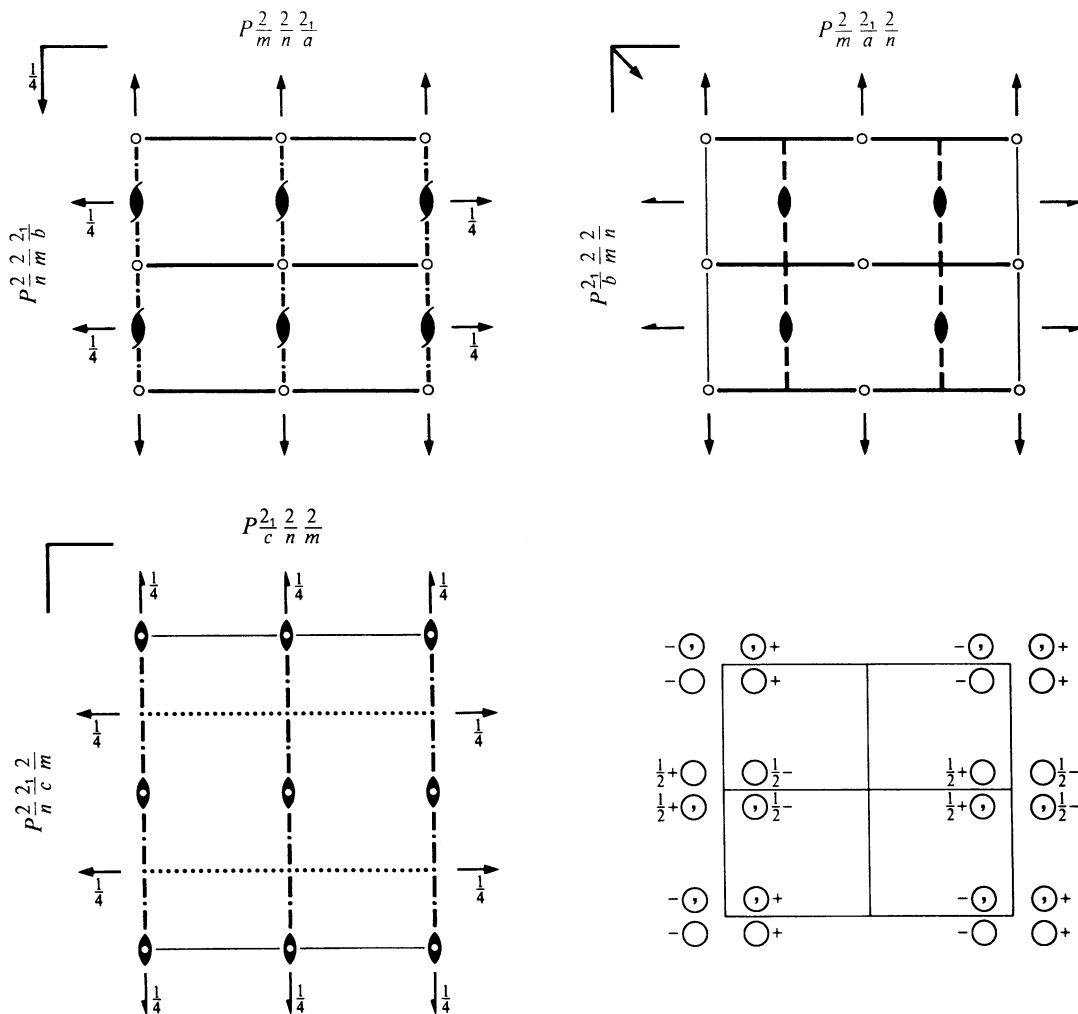
mmm

Orthorhombic

No. 53

$P 2/m 2/n 2_1/a$

Patterson symmetry $Pmmm$



Origin at centre ($2/m$) at $2/mn1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|-------------------------|--|--|-----------------|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2 \frac{1}{4}, y, \frac{1}{4}$ | (4) $2 x, 0, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) $a x, y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (8) $m 0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>i</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (4) x, \bar{y}, \bar{z} (5) $\bar{x}, \bar{y}, \bar{z}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (8) \bar{x}, y, z	General: $h0l : h + l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>h</i> $m..$	$0, y, z$ $\frac{1}{2}, \bar{y}, z + \frac{1}{2}$ $\frac{1}{2}, y, \bar{z} + \frac{1}{2}$ $0, \bar{y}, \bar{z}$	no extra conditions
4 <i>g</i> $.2.$	$\frac{1}{4}, y, \frac{1}{4}$ $\frac{1}{4}, \bar{y}, \frac{3}{4}$ $\frac{3}{4}, \bar{y}, \frac{3}{4}$ $\frac{3}{4}, y, \frac{1}{4}$	$hkl : h = 2n$
4 <i>f</i> $2..$	$x, \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \frac{1}{2}, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + l = 2n$
4 <i>e</i> $2..$	$x, 0, 0$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $\bar{x}, 0, 0$ $x + \frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + l = 2n$
2 <i>d</i> $2/m..$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + l = 2n$
2 <i>c</i> $2/m..$	$\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + l = 2n$
2 <i>b</i> $2/m..$	$\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : h + l = 2n$
2 <i>a</i> $2/m..$	$0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + l = 2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pmn2_1$ (31)	1; 2; 7; 8
	[2] $P2na$ ($Pnc2$, 30)	1; 4; 6; 7
	[2] $Pm2a$ ($Pma2$, 28)	1; 3; 6; 8
	[2] $P222_1$ (17)	1; 2; 3; 4
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/m11$ ($P2/m$, 10)	1; 4; 5; 8

IIa none

IIb [2] $Pbna$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pbcn$, 60); [2] $Pmnn$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pnmm$, 58); [2] $Pbnn$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pnna$, 52)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmna$ ($\mathbf{b}' = 2\mathbf{b}$) (53); [3] $Pmna$ ($\mathbf{a}' = 3\mathbf{a}$) (53); [3] $Pmna$ ($\mathbf{c}' = 3\mathbf{c}$) (53)

Minimal non-isomorphic supergroups

I none

II [2] $Cmce$ (64); [2] $Bmmm$ ($Cmmm$, 65); [2] $Amaa$ ($Cccm$, 66); [2] $Imma$ (74); [2] $Pmaa$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pccm$, 49); [2] $Pmcm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmma$, 51)

Pcca

D_{2h}^8

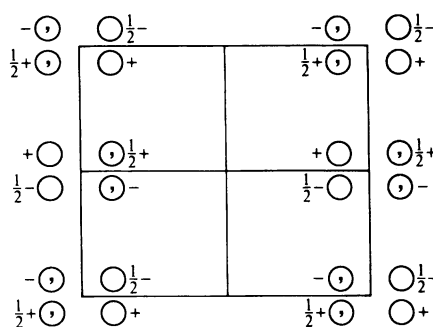
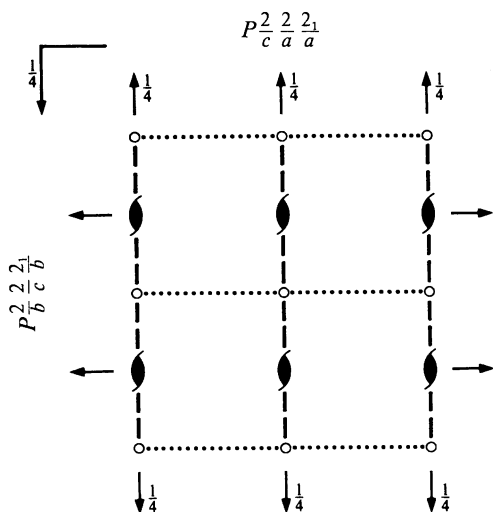
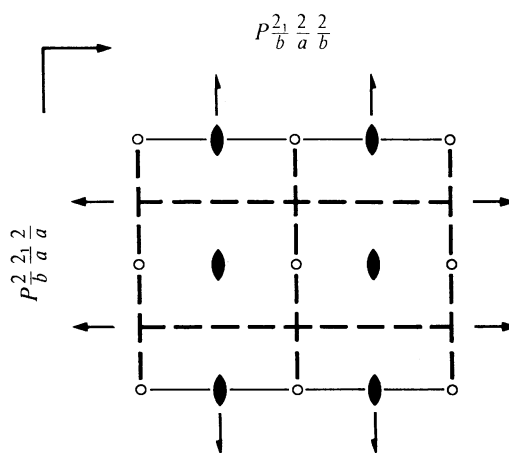
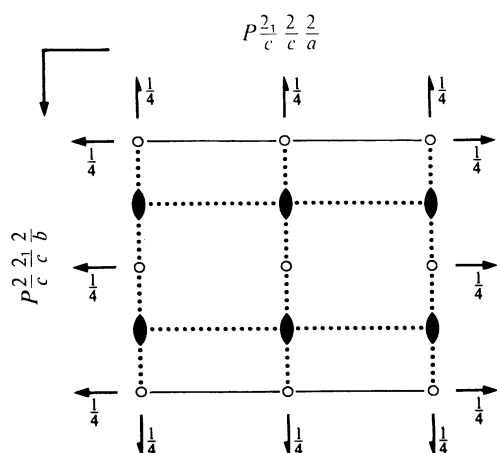
mmm

Orthorhombic

No. 54

$P 2_1/c 2/c 2/a$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1ca$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- (1) 1 (2) $2 \frac{1}{2}, 0, z$ (3) $2 0, y, \frac{1}{4}$ (4) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{4}$
 (5) $\bar{1} 0, 0, 0$ (6) $a x, y, 0$ (7) $c x, 0, z$ (8) $c \frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>f</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (6) $x + \frac{1}{2}, y, \bar{z}$	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	General: $Ok_l : l = 2n$ $h0l : l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : l = 2n$
4 <i>e</i> ..2	$\frac{1}{4}, \frac{1}{2}, z$	$\frac{3}{4}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{2}, \bar{z}$	$\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>d</i> ..2	$\frac{1}{4}, 0, z$	$\frac{3}{4}, 0, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, 0, \bar{z}$	$\frac{1}{4}, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>c</i> .2.	$0, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$	$\frac{1}{2}, y, \frac{3}{4}$	$hkl : h + l = 2n$
4 <i>b</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h, l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h, l = 2n$

Symmetry of special projections

Along [001] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x, 0, 0

Along [010] $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at 0, y, 0

Maximal non-isomorphic subgroups

I	[2] $Pc2a$ ($Pba2$, 32)	1; 3; 6; 8
	[2] $P2_1ca$ ($Pca2_1$, 29)	1; 4; 6; 7
	[2] $Pcc2$ (27)	1; 2; 7; 8
	[2] $P2_122$ ($P222_1$, 17)	1; 2; 3; 4
	[2] $P2_1/c11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P112/a$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7

IIa none

IIb [2] $Pnca$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pbcn$, 60); [2] $Pccn$ ($\mathbf{b}' = 2\mathbf{b}$) (56); [2] $Pncn$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pnna$, 52)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pcca$ ($\mathbf{b}' = 2\mathbf{b}$) (54); [3] $Pcca$ ($\mathbf{a}' = 3\mathbf{a}$) (54); [3] $Pcca$ ($\mathbf{c}' = 3\mathbf{c}$) (54)

Minimal non-isomorphic supergroups

I none

II [2] $Aema$ ($Cmce$, 64); [2] $Bmem$ ($Cmme$, 67); [2] $Ccce$ (68); [2] $Ibca$ (73); [2] $Pccm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (49); [2] $Pmma$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (51)

Pbam

D_{2h}^9

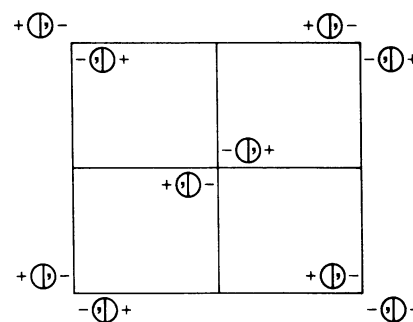
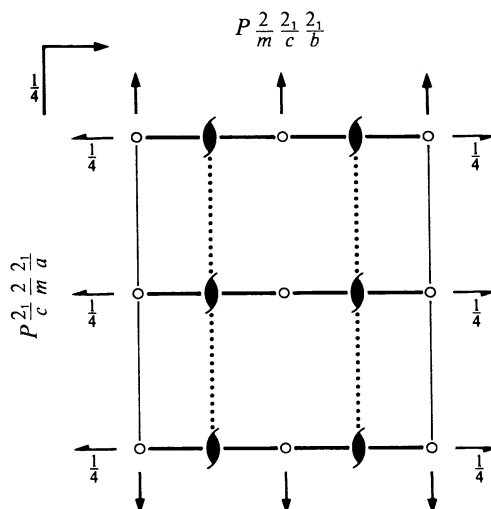
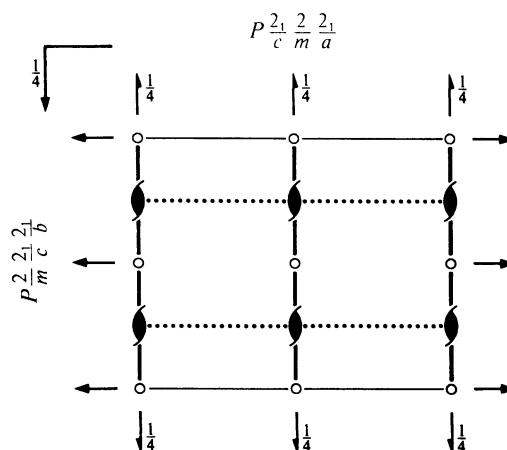
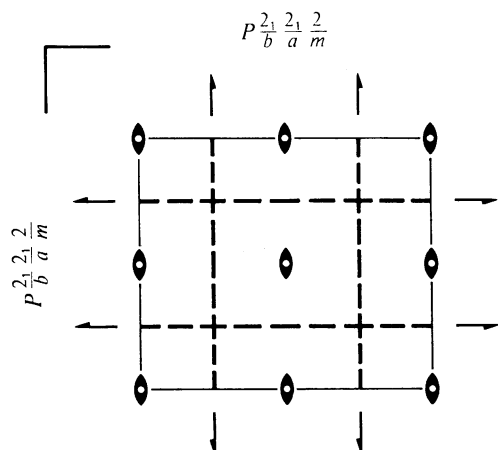
mmm

Orthorhombic

No. 55

$P 2_1/b 2_1/a 2/m$

Patterson symmetry $Pmmm$



Origin at centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------|-------------------|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) m $x, y, 0$ | (7) a $x, \frac{1}{4}, z$ | (8) b $\frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>i</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	General: $0kl : k = 2n$ $h0l : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ Special: as above, plus
4 <i>h</i> .. <i>m</i>	$x, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>g</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	no extra conditions
4 <i>f</i> .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$	$hkl : h + k = 2n$
4 <i>e</i> .. 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hkl : h + k = 2n$
2 <i>d</i> .. $2/m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>c</i> .. $2/m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : h + k = 2n$
2 <i>b</i> .. $2/m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> .. $2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I [2] $Pba2$ (32) 1; 2; 7; 8
[2] $Pb2_1m$ ($Pmc2_1$, 26) 1; 3; 6; 8
[2] $P2_1am$ ($Pmc2_1$, 26) 1; 4; 6; 7
[2] $P2_12_12$ (18) 1; 2; 3; 4
[2] $P12_1/a1$ ($P2_1/c$, 14) 1; 3; 5; 7
[2] $P2_1/b11$ ($P2_1/c$, 14) 1; 4; 5; 8
[2] $P112/m$ ($P2/m$, 10) 1; 2; 5; 6

IIa none

IIb [2] $Pnam$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnma$, 62); [2] $Pbnm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnma$, 62); [2] $Pnnm$ ($\mathbf{c}' = 2\mathbf{c}$) (58)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pbam$ ($\mathbf{c}' = 2\mathbf{c}$) (55); [3] $Pbam$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (55)

Minimal non-isomorphic supergroups

I [2] $P4/mbm$ (127); [2] $P4_2/mbc$ (135)

II [2] $Aeam$ ($Cmce$, 64); [2] $Bbem$ ($Cmce$, 64); [2] $Cmmm$ (65); [2] $Ibam$ (72); [2] $Pbmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmma$, 51);
[2] $Pmam$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmma$, 51)

Pccn

D_{2h}^{10}

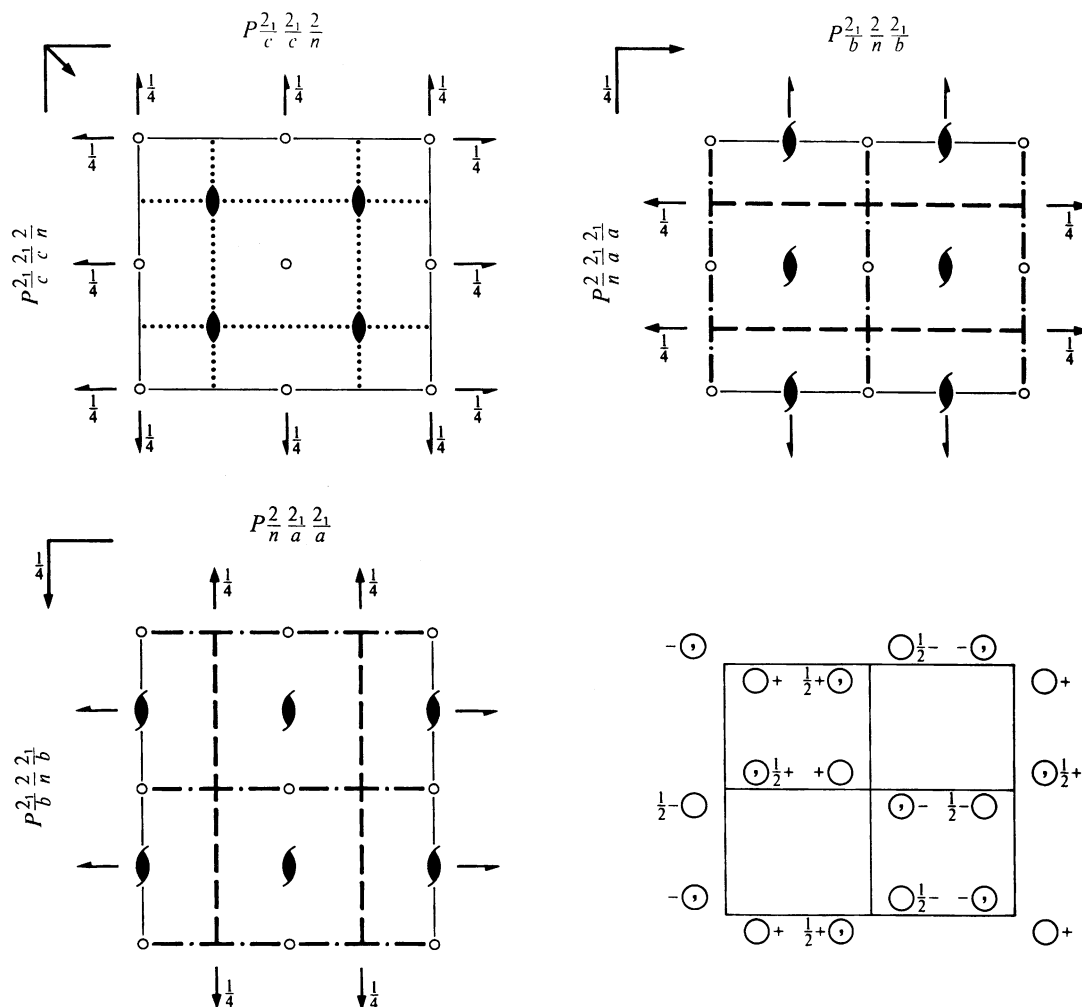
mmm

Orthorhombic

No. 56

$P 2_1/c 2_1/c 2/n$

Patterson symmetry *Pmmm*



Origin at $\bar{1}$ on $11n$

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------------|--|--|--|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{4}$ |
| (5) $\bar{1} \quad 0, 0, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, 0$ | (7) $c \quad x, \frac{1}{4}, z$ | (8) $c \quad \frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>e</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	General: $0kl : l = 2n$ $h0l : l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : l = 2n$ $hkl : l = 2n$ $hkl : h + k, h + l, k + l = 2n$ $hkl : h + k, h + l, k + l = 2n$
4 <i>d</i> .. 2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>c</i> .. 2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pc2_1n$ ($Pna2_1, 33$)	1; 3; 6; 8
	[2] $P2_1cn$ ($Pna2_1, 33$)	1; 4; 6; 7
	[2] $Pcc2$ (27)	1; 2; 7; 8
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/c1$ ($P2_1/c, 14$)	1; 3; 5; 7
	[2] $P2_1/c11$ ($P2_1/c, 14$)	1; 4; 5; 8
	[2] $P112/n$ ($P2/c, 13$)	1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pccn$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (56); [3] $Pccn$ ($\mathbf{c}' = 3\mathbf{c}$) (56)

Minimal non-isomorphic supergroups

I [2] $P4/ncc$ (130); [2] $P4_2/ncm$ (138)

II [2] $Aema$ ($Cmce, 64$); [2] $Bmeb$ ($Cmce, 64$); [2] $Cccm$ (66); [2] $Ibam$ (72); [2] $Pccb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pcca, 54$); [2] $Pcca$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (54); [2] $Pmmn$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (59)

$Pbcm$

D_{2h}^{11}

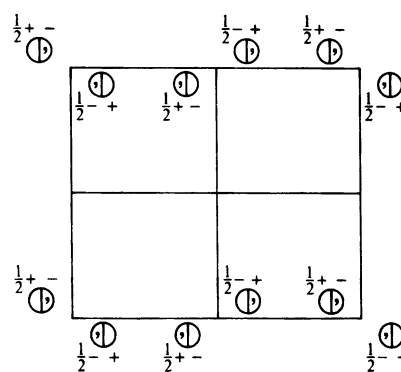
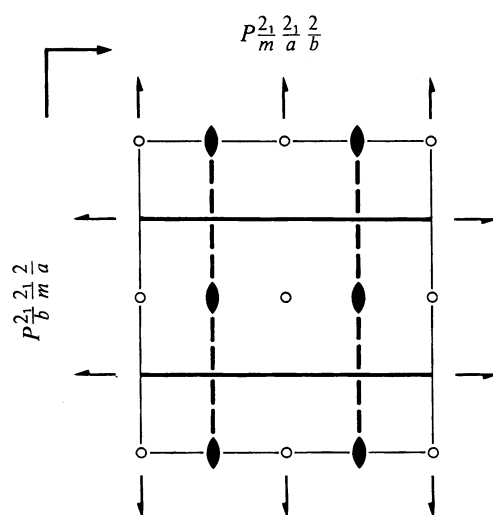
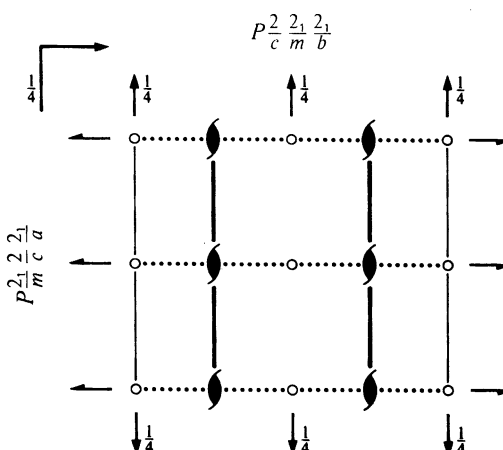
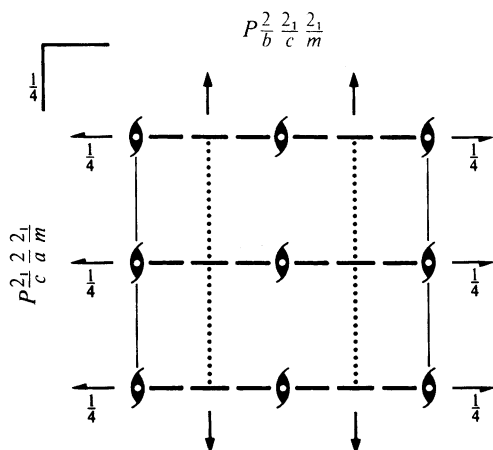
mmm

Orthorhombic

No. 57

$P 2/b 2_1/c 2_1/m$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $b12_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|-------------------------|--------------------------------------|--|-----------------------------|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) 2 $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) m $x, y, \frac{1}{4}$ | (7) c $x, \frac{1}{4}, z$ | (8) b $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>e</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (6) $x, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x}, y + \frac{1}{2}, z$	General: $0kl : k = 2n$ $h0l : l = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>d</i> $\dots m$	$x, y, \frac{1}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$	$\bar{x}, y + \frac{1}{2}, \frac{1}{4}$	$x, \bar{y} + \frac{1}{2}, \frac{3}{4}$	no extra conditions
4 <i>c</i> $2 \dots$	$x, \frac{1}{4}, 0$	$\bar{x}, \frac{3}{4}, \frac{1}{2}$	$\bar{x}, \frac{1}{4}, 0$	$x, \frac{1}{4}, \frac{1}{2}$	$hkl : l = 2n$
4 <i>b</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : k, l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$hkl : k, l = 2n$

Symmetry of special projections

Along [001] $p2gm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at x, 0, 0

Along [010] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at 0, y, 0

Maximal non-isomorphic subgroups

I	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $P2cm$ ($Pma2$, 28)	1; 4; 6; 7
	[2] $Pb2_1m$ ($Pmc2_1$, 26)	1; 3; 6; 8
	[2] $P22_12_1$ ($P2_12_12_1$, 18)	1; 2; 3; 4
	[2] $P12_1/c1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2/b11$ ($P2/c$, 13)	1; 4; 5; 8
	[2] $P112_1/m$ ($P2_1/m$, 11)	1; 2; 5; 6

IIa none

IIb [2] $Pbnm$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pnma$, 62); [2] $Pbca$ ($\mathbf{a}' = 2\mathbf{a}$) (61); [2] $Pbna$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pbcn$, 60)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pbcm$ ($\mathbf{a}' = 2\mathbf{a}$) (57); [3] $Pbcm$ ($\mathbf{b}' = 3\mathbf{b}$) (57); [3] $Pbcm$ ($\mathbf{c}' = 3\mathbf{c}$) (57)

Minimal non-isomorphic supergroups

I none

II [2] $Cmcm$ (63); [2] $Bbem$ ($Cmce$, 64); [2] $Aemm$ ($Cmme$, 67); [2] $Ibam$ (72); [2] $Pmcm$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Pbmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pmma$, 51)

$Pn\bar{1}m$

D_{2h}^{12}

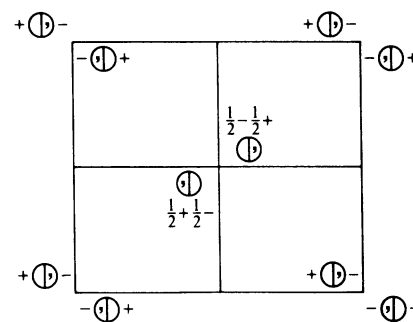
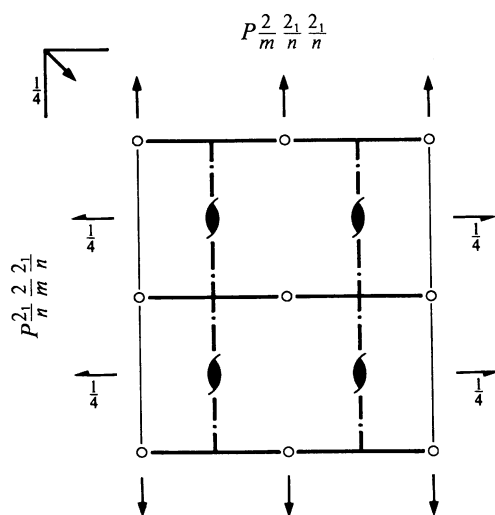
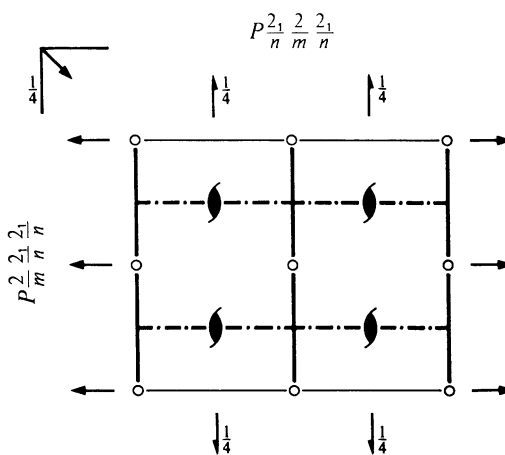
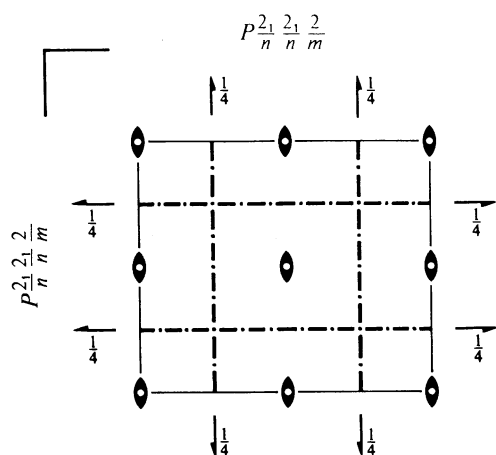
mmm

Orthorhombic

No. 58

$P 2_1/n 2_1/n 2/m$

Patterson symmetry $Pmmm$



Origin at centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------|-------------------|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) m $x, y, 0$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>h</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	General: $Ok\bar{l} : k + l = 2n$ $h0l : h + l = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>g</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>f</i> .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>e</i> .. 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
2 <i>d</i> .. $2/m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl : h + k + l = 2n$
2 <i>c</i> .. $2/m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2 <i>b</i> .. $2/m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2 <i>a</i> .. $2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[010]$ $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2_1m$ ($Pmn2_1$, 31)	1; 3; 6; 8
	[2] $P2_1nm$ ($Pmn2_1$, 31)	1; 4; 6; 7
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/n1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2_1/n11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnmm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (58); [3] $Pnmm$ ($\mathbf{c}' = 3\mathbf{c}$) (58)

Minimal non-isomorphic supergroups

I	[2] $P4/mnc$ (128); [2] $P4_2/mnm$ (136)
II	[2] $Amam$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Cccm$ (66); [2] $Immm$ (71); [2] $Pncm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmna$, 53); [2] $Pcnm$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmna$, 53); [2] $Pbam$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (55)

$Pmmn$

D_{2h}^{13}

mmm

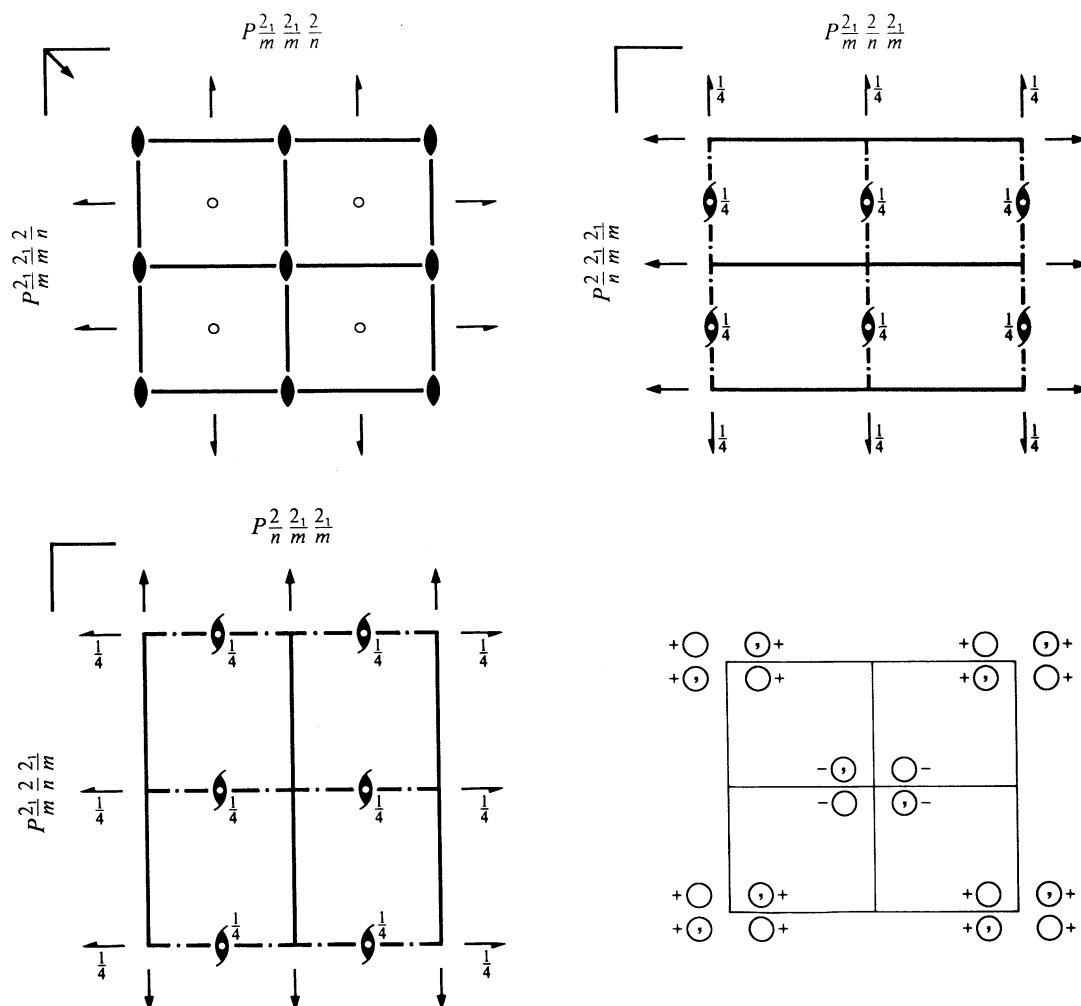
Orthorhombic

No. 59

$P 2_1/m 2_1/m 2/n$

Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $mm2/n$, at $\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---|--|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (7) m $x, 0, z$ | (8) m $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) x, \bar{y}, z	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) \bar{x}, y, z	$hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$
					Special: as above, plus
4 <i>f</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \bar{z}$	$x + \frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
4 <i>e</i> <i>m</i> ..	$0, y, z$	$0, \bar{y}, z$	$\frac{1}{2}, y + \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>c</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h, k = 2n$
2 <i>b</i> <i>m m</i> 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
2 <i>a</i> <i>m m</i> 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions

Symmetry of special projections

Along [001] *c*2*m m*

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, *z*

Along [100] *p*2*m g*

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $\frac{1}{4}, \frac{1}{4}, 0$

Along [010] *p*2*g m*

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $\frac{1}{4}, y, 0$

Maximal non-isomorphic subgroups

I	[2] <i>Pm</i> 2 ₁ <i>n</i> (<i>Pmn</i> 2 ₁ , 31)	1; 3; 6; 8
	[2] <i>P</i> 2 ₁ <i>mn</i> (<i>Pmn</i> 2 ₁ , 31)	1; 4; 6; 7
	[2] <i>Pmm</i> 2 (25)	1; 2; 7; 8
	[2] <i>P</i> 2 ₁ 2 ₁ 2 (18)	1; 2; 3; 4
	[2] <i>P</i> 112/ <i>n</i> (<i>P</i> 2/ <i>c</i> , 13)	1; 2; 5; 6
	[2] <i>P</i> 12 ₁ / <i>m</i> 1 (<i>P</i> 2 ₁ / <i>m</i> , 11)	1; 3; 5; 7
	[2] <i>P</i> 2 ₁ / <i>m</i> 11 (<i>P</i> 2 ₁ / <i>m</i> , 11)	1; 4; 5; 8

IIa none

IIb [2] *Pcmn* ($\mathbf{c}' = 2\mathbf{c}$) (*Pnma*, 62); [2] *Pm \bar{c} n* ($\mathbf{c}' = 2\mathbf{c}$) (*Pnma*, 62); [2] *Pccn* ($\mathbf{c}' = 2\mathbf{c}$) (56)

Maximal isomorphic subgroups of lowest index

IIc [2] *Pmmn* ($\mathbf{c}' = 2\mathbf{c}$) (59); [3] *Pmmn* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

I [2] *P*4/*nmm* (129); [2] *P*4₂/*nmc* (137)

II [2] *A**m**m**a* (*Cmcm*, 63); [2] *B**m**m**b* (*Cmcm*, 63); [2] *C**m**m**m* (65); [2] *I**m**m**m* (71); [2] *P**m**m**b* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Pmma*, 51); [2] *P**m**m**a* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (51)

$Pmmn$

D_{2h}^{13}

mmm

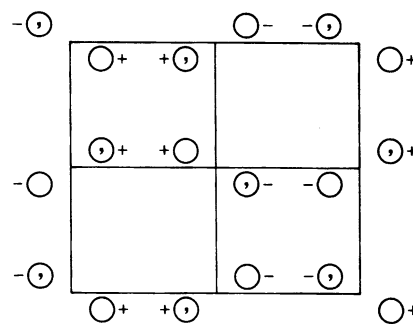
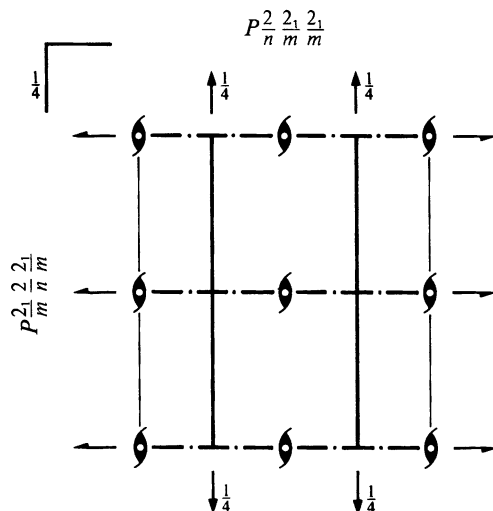
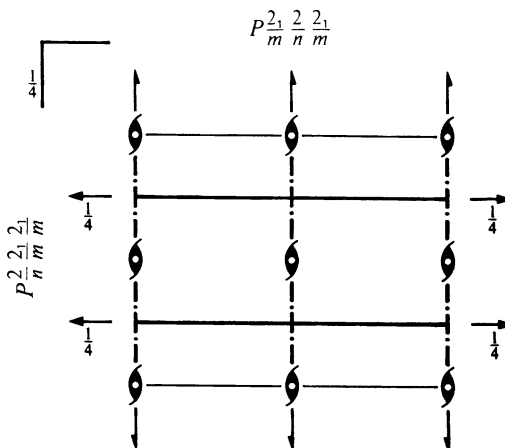
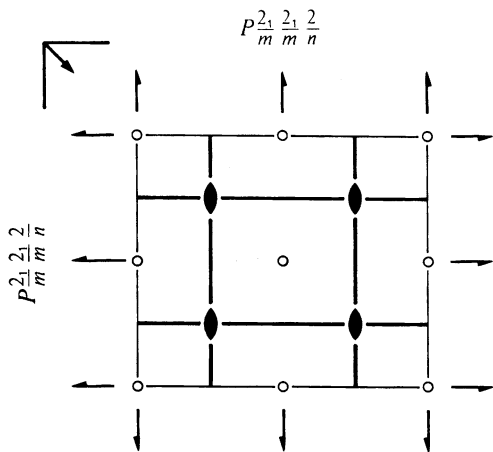
Orthorhombic

No. 59

$P 2_1/m 2_1/m 2/n$

Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $2_1 2_1 n$, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from $mm2$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1
- (2) $2 \frac{1}{4}, \frac{1}{4}, z$
- (3) $2(0, \frac{1}{2}, 0) 0, y, 0$
- (4) $2(\frac{1}{2}, 0, 0) x, 0, 0$
- (5) $\bar{1} 0, 0, 0$
- (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$
- (7) $m x, \frac{1}{4}, z$
- (8) $m \frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>g</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (7) $x, \bar{y} + \frac{1}{2}, z$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y, z$	General: $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ Special: as above, plus
4 <i>f</i> . <i>m</i> .	$x, \frac{1}{4}, z$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, z$	$\bar{x}, \frac{3}{4}, \bar{z}$	$x + \frac{1}{2}, \frac{3}{4}, \bar{z}$	no extra conditions
4 <i>e</i> <i>m</i> ..	$\frac{1}{4}, y, z$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, z$	$\frac{3}{4}, y + \frac{1}{2}, \bar{z}$	$\frac{3}{4}, \bar{y}, \bar{z}$	no extra conditions
4 <i>d</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>c</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h, k = 2n$
2 <i>b</i> <i>m m</i> 2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$			no extra conditions
2 <i>a</i> <i>m m</i> 2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$			no extra conditions

Symmetry of special projections

Along [001] *c*2*m m*

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] *p*2*m g*

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [010] *p*2*g m*

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] <i>Pm</i> 2 ₁ <i>n</i> (<i>Pmn</i> 2 ₁ , 31)	1; 3; 6; 8
	[2] <i>P</i> 2 ₁ <i>mn</i> (<i>Pmn</i> 2 ₁ , 31)	1; 4; 6; 7
	[2] <i>Pmm</i> 2 (25)	1; 2; 7; 8
	[2] <i>P</i> 2 ₁ 2 ₁ 2 (18)	1; 2; 3; 4
	[2] <i>P</i> 112/ <i>n</i> (<i>P</i> 2/ <i>c</i> , 13)	1; 2; 5; 6
	[2] <i>P</i> 12 ₁ / <i>m</i> 1 (<i>P</i> 2 ₁ / <i>m</i> , 11)	1; 3; 5; 7
	[2] <i>P</i> 2 ₁ / <i>m</i> 11 (<i>P</i> 2 ₁ / <i>m</i> , 11)	1; 4; 5; 8

IIa none

IIb [2] *Pcmn* ($\mathbf{c}' = 2\mathbf{c}$) (*Pnma*, 62); [2] *Pm₂cn* ($\mathbf{c}' = 2\mathbf{c}$) (*Pnma*, 62); [2] *Pccn* ($\mathbf{c}' = 2\mathbf{c}$) (56)

Maximal isomorphic subgroups of lowest index

IIc [2] *Pmmn* ($\mathbf{c}' = 2\mathbf{c}$) (59); [3] *Pmmn* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

I [2] *P*4/*nmm* (129); [2] *P*4₂/*nmc* (137)

II [2] *A**m**m**a* (*Cmcm*, 63); [2] *B**m**m**b* (*Cmcm*, 63); [2] *C**m**m**m* (65); [2] *I**m**m**m* (71); [2] *P**m**m**b* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Pmma*, 51); [2] *P**m**m**a* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (51)

$Pbcn$

D_{2h}^{14}

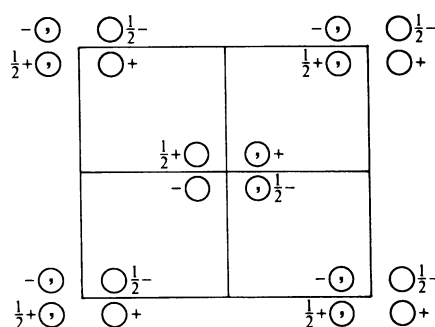
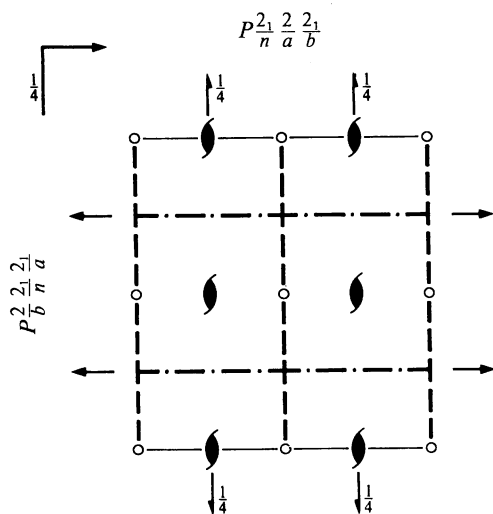
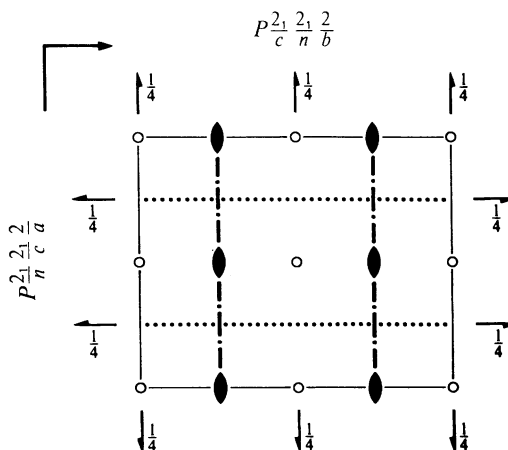
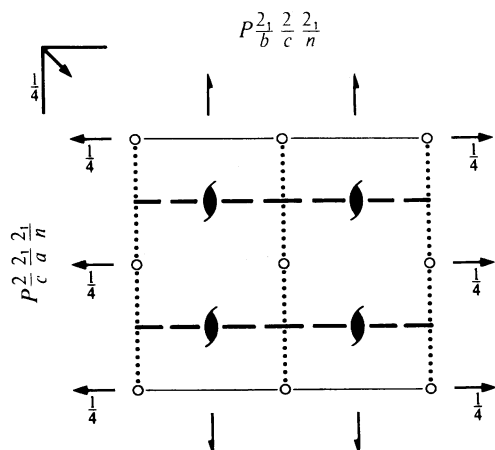
mmm

Orthorhombic

No. 60

$P 2_1/b 2/c 2_1/n$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1c1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------|--|----------------------------|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, y, \frac{1}{4})$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (7) c $x, 0, z$ | (8) b $\frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>d</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$Ok\bar{l} : k = 2n$
	(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(7) $x, \bar{y}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	$h0\bar{l} : l = 2n$
					$hk0 : h + k = 2n$
					$h00 : h = 2n$
					$0k0 : k = 2n$
					$00\bar{l} : l = 2n$
					Special: as above, plus
4 <i>c</i> .2.	$0, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{3}{4}$	$0, \bar{y}, \frac{3}{4}$	$\frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k = 2n$
4 <i>b</i> $\bar{1}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along $[001]$ $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along $[100]$ $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along $[010]$ $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $P2_1cn$ ($Pna2_1$, 33)	1; 4; 6; 7
	[2] $Pb2n$ ($Pnc2$, 30)	1; 3; 6; 8
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $P2_12_2$ ($P2_12_1$, 18)	1; 2; 3; 4
	[2] $P112_1/n$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/b11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pbcn$ ($\mathbf{a}' = 3\mathbf{a}$) (60); [3] $Pbcn$ ($\mathbf{b}' = 3\mathbf{b}$) (60); [3] $Pbcn$ ($\mathbf{c}' = 3\mathbf{c}$) (60)

Minimal non-isomorphic supergroups

I none

II [2] $Cmcm$ (63); [2] $Aema$ ($Cmce$, 64); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmn$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pmna$, 53);

[2] $Pbcb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pcca$, 54); [2] $Pmca$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pbcm$, 57)

Pbca

D_{2h}^{15}

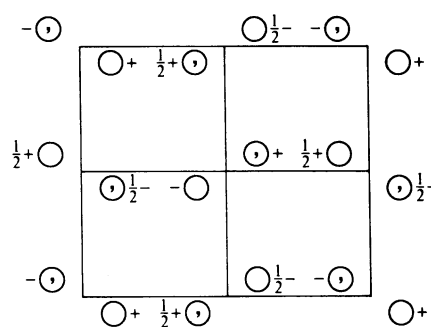
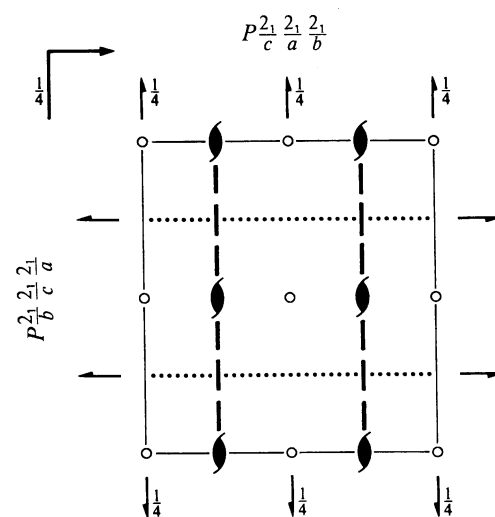
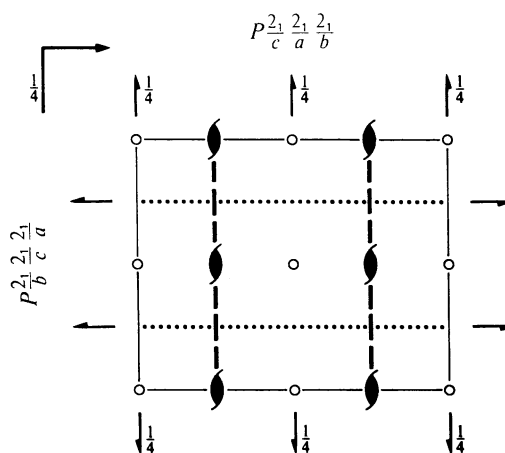
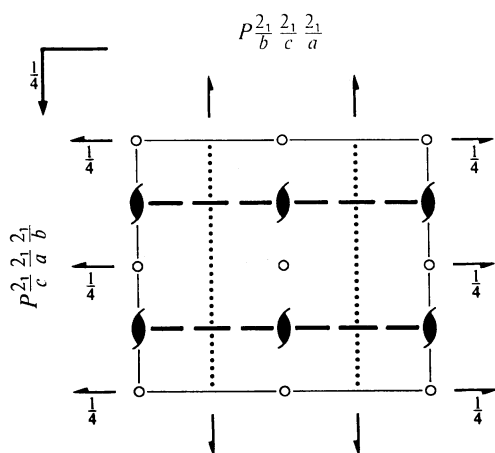
mmm

Orthorhombic

No. 61

$P 2_1/b 2_1/c 2_1/a$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------|--|--|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) a $x, y, \frac{1}{4}$ | (7) c $x, \frac{1}{4}, z$ | (8) b $\frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>c</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	General: $Ok\bar{l} : k = 2n$ $h0l : l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : h + k, h + l, k + l = 2n$ $hkl : h + k, h + l, k + l = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$

Symmetry of special projections

Along [001] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, 0, 0

Along [010] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0, y, 0

Maximal non-isomorphic subgroups

I	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $Pb2_1a$ ($Pca2_1$, 29)	1; 3; 6; 8
	[2] $P2_1ca$ ($Pca2_1$, 29)	1; 4; 6; 7
	[2] $P2_12_12_1$ (19)	1; 2; 3; 4
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P12_1/c1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2_1/b11$ ($P2_1/c$, 14)	1; 4; 5; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pbca$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (61)

Minimal non-isomorphic supergroups

I [3] $Pa\bar{3}$ (205)

II [2] $Aema$ ($Cmce$, 64); [2] $Bbem$ ($Cmce$, 64); [2] $Cmce$ (64); [2] $Ibca$ (73); [2] $Pbcm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (57);
 [2] $Pmca$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pbcm$, 57); [2] $Pbma$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pbcm$, 57)

Pnma

D_{2h}^{16}

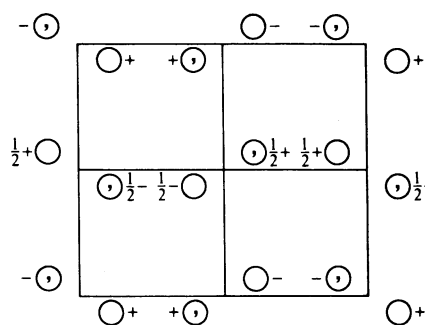
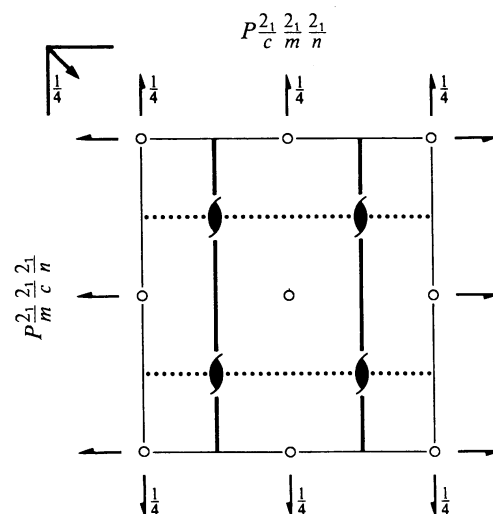
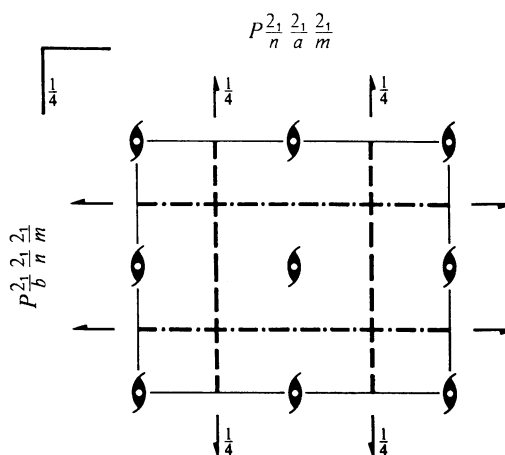
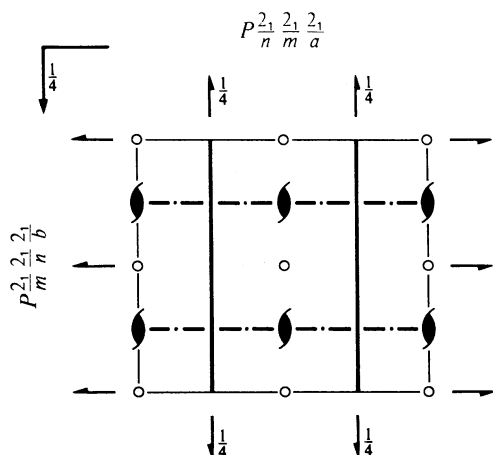
mmm

Orthorhombic

No. 62

$P 2_1/n 2_1/m 2_1/a$

Patterson symmetry *Pmmm*



Origin at $\bar{1}$ on 12,1

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$

Symmetry operations

- | | | | |
|-----------------------------|--|--|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1} \quad 0, 0, 0$ | (6) $a \quad x, y, \frac{1}{4}$ | (7) $m \quad x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>d</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (7) $x, \bar{y} + \frac{1}{2}, z$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	General: $0kl : k + l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
4 <i>c</i> . <i>m</i> .	$x, \frac{1}{4}, z$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}$	$\bar{x}, \frac{3}{4}, \bar{z}$	$x + \frac{1}{2}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	no extra conditions
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + l, k = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + l, k = 2n$

Symmetry of special projections

Along [001] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [010] $p2gg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pn2_1a$ ($Pna2_1$, 33)	1; 3; 6; 8
	[2] $Pnm2_1$ ($Pmn2_1$, 31)	1; 2; 7; 8
	[2] $P2_1ma$ ($Pmc2_1$, 26)	1; 4; 6; 7
	[2] $P2_12_12_1$ (19)	1; 2; 3; 4
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/n11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12_1/m1$ ($P2_1/m$, 11)	1; 3; 5; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnma$ ($\mathbf{a}' = 3\mathbf{a}$) (62); [3] $Pnma$ ($\mathbf{b}' = 3\mathbf{b}$) (62); [3] $Pnma$ ($\mathbf{c}' = 3\mathbf{c}$) (62)

Minimal non-isomorphic supergroups

I none

II [2] $Amma$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Ccme$ ($Cmce$, 64); [2] $Imma$ (74); [2] $Pcma$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pbam$, 55); [2] $Pbma$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pbcm$, 57); [2] $Pnmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmnn$, 59)

$Cmcm$

D_{2h}^{17}

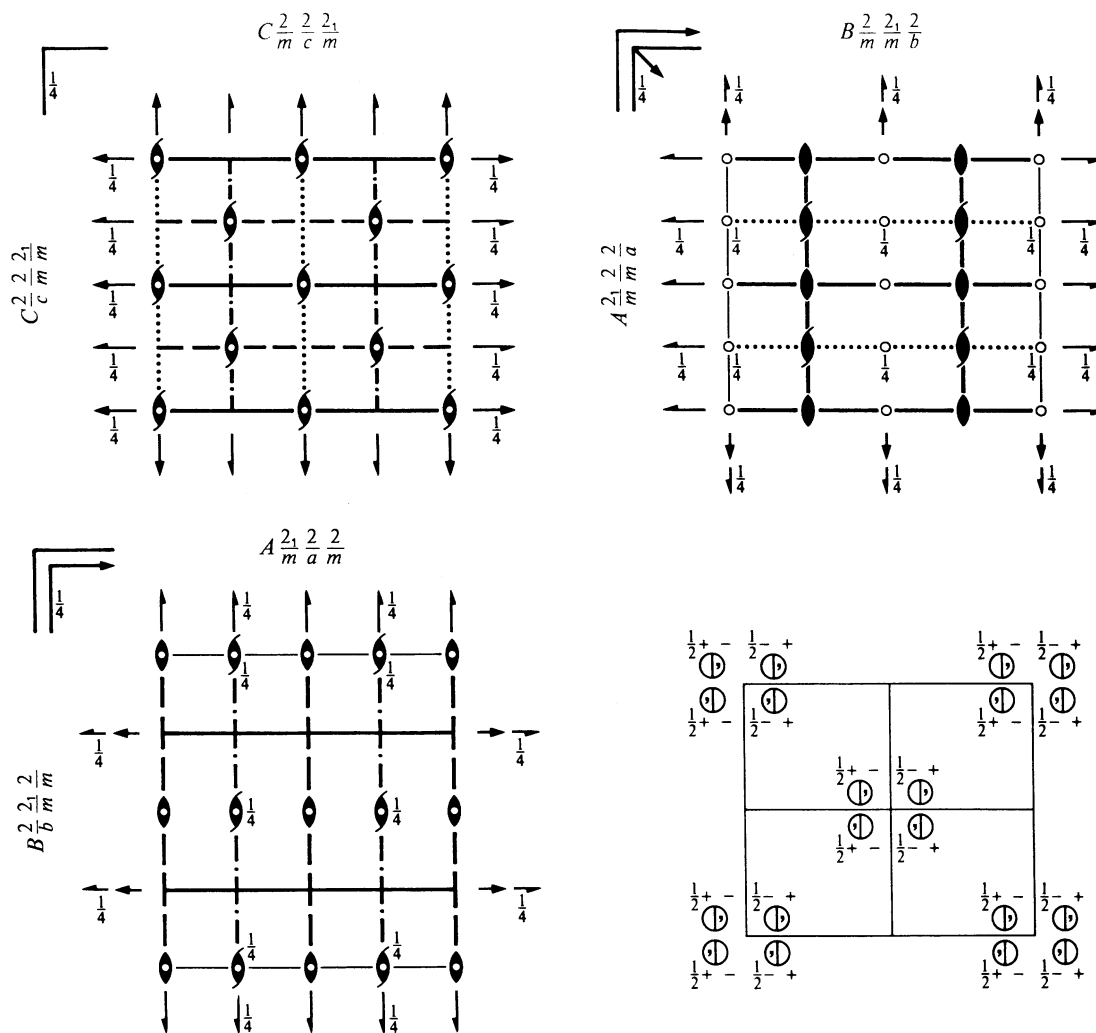
mmm

Orthorhombic

No. 63

$C 2/m 2/c 2_1/m$

Patterson symmetry $Cmmm$



Origin at centre $(2/m)$ at $2/mc2_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---------------------|----------------------------------|-------------------------|---------------|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,0,z$ | (3) $2 0,y,\frac{1}{4}$ | (4) $2 x,0,0$ |
| (5) $\bar{1} 0,0,0$ | (6) $m x,y,\frac{1}{4}$ | (7) $c x,0,z$ | (8) $m 0,y,z$ |

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $\bar{1} \frac{1}{4},\frac{1}{4},0$ | (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$ | (7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ | (8) $b \frac{1}{4},y,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
16 <i>h</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x},\bar{y},z+\frac{1}{2}$ (6) $x,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) x,\bar{y},\bar{z} (8) \bar{x},y,z	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h,l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8 <i>g</i> .. <i>m</i>	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$\bar{x},y,\frac{1}{4}$	$x,\bar{y},\frac{3}{4}$	no extra conditions
8 <i>f</i> <i>m</i> ..	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$	$0,y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8 <i>e</i> 2..	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$\bar{x},0,0$	$x,0,\frac{1}{2}$	$hkl : l=2n$
8 <i>d</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$hkl : k,l=2n$
4 <i>c</i> <i>m</i> 2 <i>m</i>	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4 <i>b</i> 2/ <i>m</i> ..	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : l=2n$
4 <i>a</i> 2/ <i>m</i> ..	$0,0,0$	$0,0,\frac{1}{2}$			$hkl : l=2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0,0,z

Along [100] $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at x,0,0

Along [010] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C2cm$ ($Ama2$, 40)	(1; 4; 6; 7)+
	[2] $Cm2m$ ($Amm2$, 38)	(1; 3; 6; 8)+
	[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+
	[2] $C222_1$ (20)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
	[2] $C112_1/m$ ($P2_1/m$, 11)	(1; 2; 5; 6)+
IIa	[2] $Pbnm$ ($Pnma$, 62)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcn$ ($Pnma$, 62)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbcn$ (60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmnm$ ($Pmnm$, 59)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmnn$ ($Pnmm$, 58)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbcm$ (57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbnn$ ($Pnna$, 52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcm$ ($Pmma$, 51)	1; 2; 3; 4; 5; 6; 7; 8

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmcm$ ($\mathbf{a}' = 3\mathbf{a}$) (63); [3] $Cmcm$ ($\mathbf{b}' = 3\mathbf{b}$) (63); [3] $Cmcm$ ($\mathbf{c}' = 3\mathbf{c}$) (63)

Minimal non-isomorphic supergroups

I [3] $P6_3/mcm$ (193); [3] $P6_3/mmc$ (194)

II [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (65)

Cmce

D_{2h}^{18}

mmm

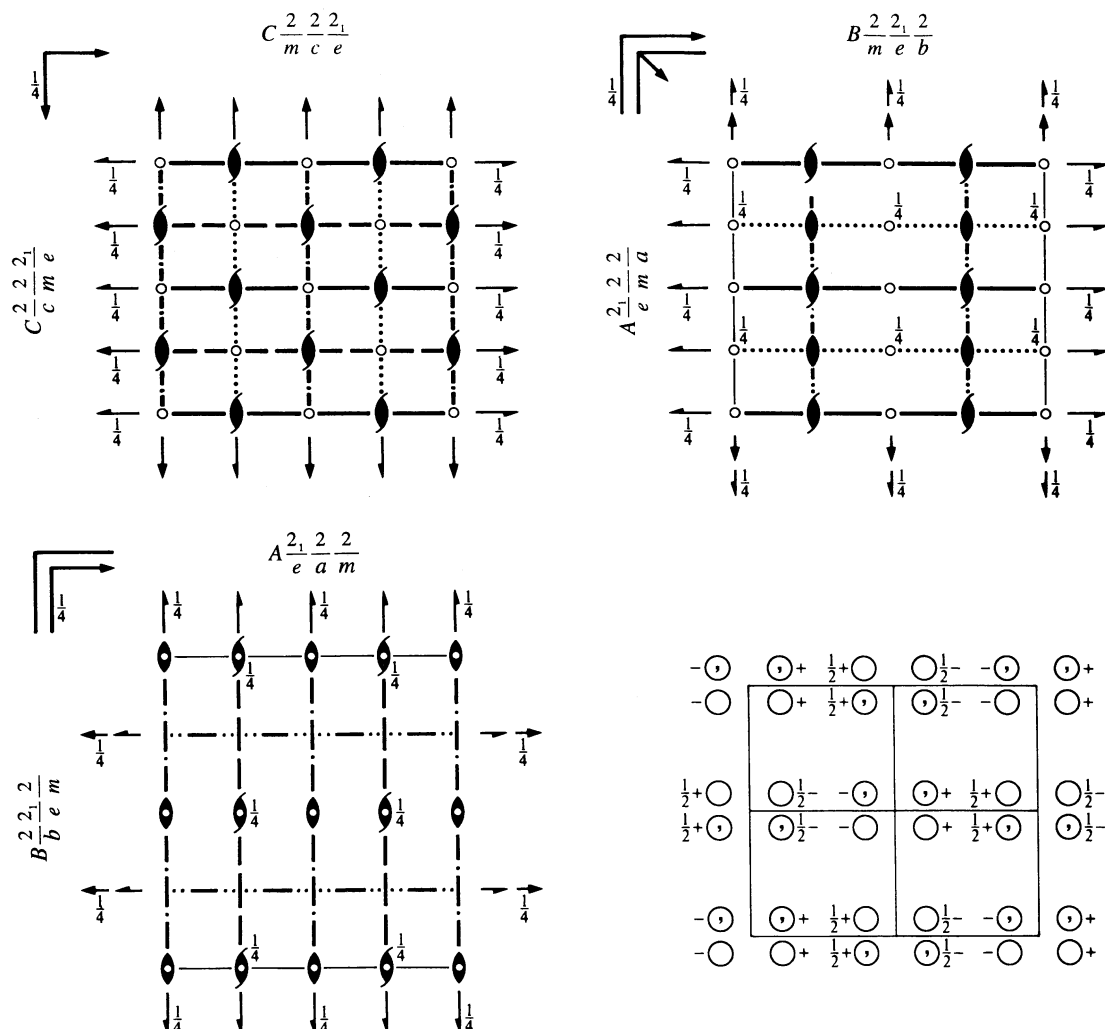
Orthorhombic

No. 64

$C 2/m 2/c 2_1/e$

Patterson symmetry *Cmmm*

Former space-group symbol *Cmca*; cf. Chapter 1.3



Origin at centre ($2/m$) at $2/mn1$

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------------|--|--|-----------------|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ | (4) 2 $x,0,0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) b $x,y,\frac{1}{4}$ | (7) c $x,\frac{1}{4},z$ | (8) m $0,y,z$ |

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ | (3) 2 $\frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ | (6) a $x,y,\frac{1}{4}$ | (7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$ | (8) b $\frac{1}{4},y,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
16	<i>g</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) x,\bar{y},\bar{z} (8) \bar{x},y,z	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8	<i>f</i> $m..$	$0,y,z$	$0,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	Special: as above, plus no extra conditions
8	<i>e</i> $.2.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{4}$	$hkl : h=2n$
8	<i>d</i> $2..$	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$	$x,\frac{1}{2},\frac{1}{2}$	$hkl : k+l=2n$
8	<i>c</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$hkl : k,l=2n$
4	<i>b</i> $2/m..$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl : k+l=2n$
4	<i>a</i> $2/m..$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0,0,z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at x,0,0

Along [010] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $C2ce$ ($Aea2$, 41)	(1; 4; 6; 7)+
	[2] $Cm2e$ ($Aem2$, 39)	(1; 3; 6; 8)+
	[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+
	[2] $C222_1$ (20)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C112_1/e$ ($P2_1/c$, 14)	(1; 2; 5; 6)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
IIa	[2] $Pmnb$ ($Pnma$, 62)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbca$ (61)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbna$ ($Pbcn$, 60)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmca$ ($Pbcm$, 57)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbnb$ ($Pccn$, 56)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcb$ ($Pbam$, 55)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pbcb$ ($Pcca$, 54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmce$ ($\mathbf{a}' = 3\mathbf{a}$) (64); [3] $Cmce$ ($\mathbf{b}' = 3\mathbf{b}$) (64); [3] $Cmce$ ($\mathbf{c}' = 3\mathbf{c}$) (64)

Minimal non-isomorphic supergroups

I none

II [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmme$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)

$Cmmm$

D_{2h}^{19}

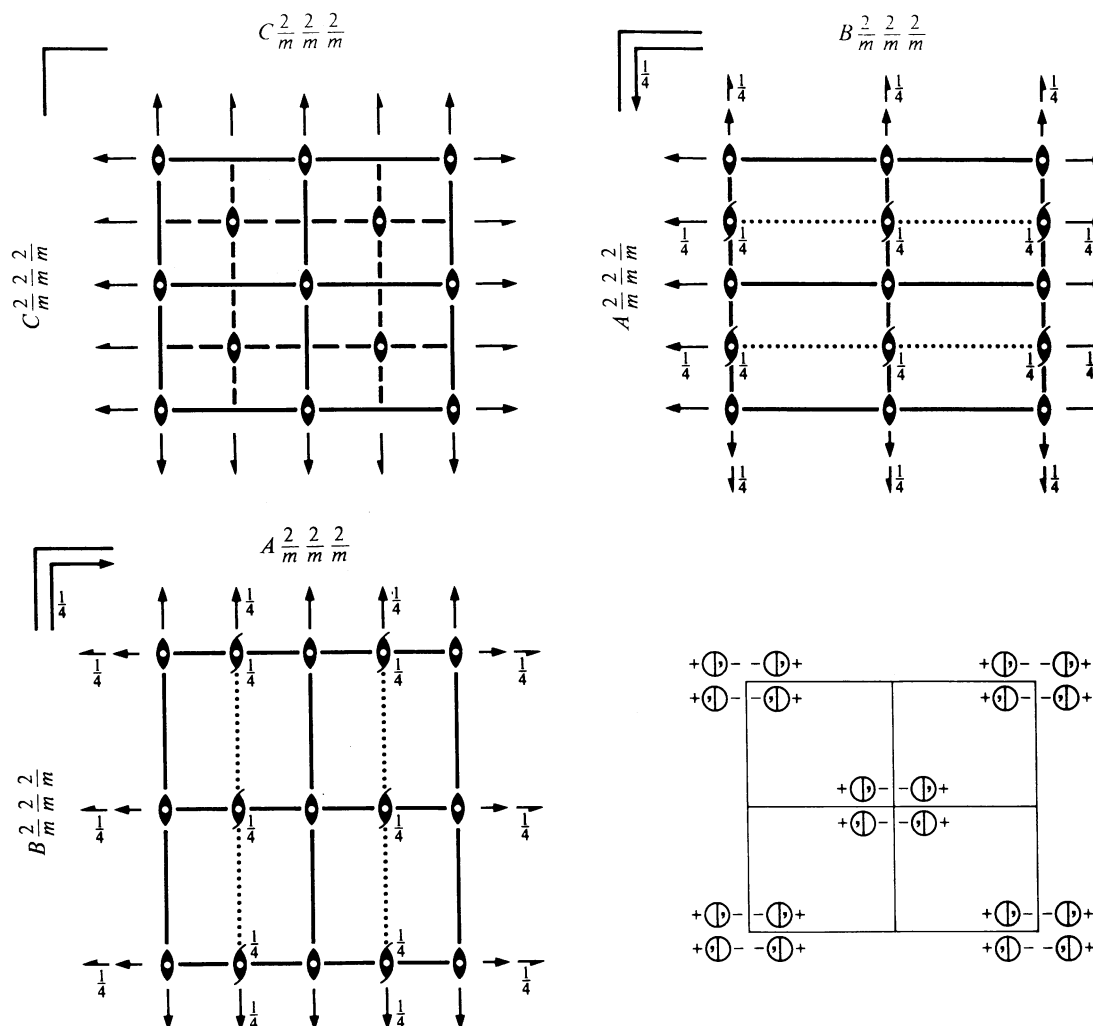
mmm

Orthorhombic

No. 65

$C 2/m 2/m 2/m$

Patterson symmetry $Cmmm$



Origin at centre (mmm)

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------------|-----------------|-----------------|-----------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) m $x,y,0$ | (7) m $x,0,z$ | (8) m $0,y,z$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|--|---|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2 $(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) 2 $(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (7) a $x, \frac{1}{4}, z$ | (8) b $\frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
16	<i>r</i>	1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) \bar{x},\bar{y},z (6) x,y,\bar{z}	(3) \bar{x},y,\bar{z} (7) x,\bar{y},z	(4) x,\bar{y},\bar{z} (8) \bar{x},y,z	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$
8	<i>q</i>	$\dots m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	Special: as above, plus no extra conditions
8	<i>p</i>	$\dots m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
8	<i>o</i>	$\dots m$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
8	<i>n</i>	$m\dots$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	<i>m</i>	$\dots 2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z$	$hkl : h=2n$
4	<i>l</i>	$mm2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	<i>k</i>	$mm2$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	<i>j</i>	$m2m$	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	<i>i</i>	$m2m$	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	<i>h</i>	$2mm$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			no extra conditions
4	<i>g</i>	$2mm$	$x,0,0$	$\bar{x},0,0$			no extra conditions
4	<i>f</i>	$\dots 2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : h=2n$
4	<i>e</i>	$\dots 2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			$hkl : h=2n$
2	<i>d</i>	mmm	$0,0,\frac{1}{2}$				no extra conditions
2	<i>c</i>	mmm	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	<i>b</i>	mmm	$\frac{1}{2},0,0$				no extra conditions
2	<i>a</i>	mmm	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0,0,z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $0,y,0$

Maximal non-isomorphic subgroups

- I** [2] $Cm2m$ ($Amm2$, 38) (1; 3; 6; 8)+
 [2] $C2mm$ ($Amm2$, 38) (1; 4; 6; 7)+
 [2] $Cmm2$ (35) (1; 2; 7; 8)+
 [2] $C222$ (21) (1; 2; 3; 4)+
 [2] $C12/m1$ ($C2/m$, 12) (1; 3; 5; 7)+
 [2] $C2/m11$ ($C2/m$, 12) (1; 4; 5; 8)+
 [2] $C112/m$ ($P2/m$, 10) (1; 2; 5; 6)+
- IIa** [2] $Pmnm$ (59) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pbam$ (55) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pbmn$ ($Pmna$, 53) 1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pman$ ($Pmna$, 53) 1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pmam$ ($Pmma$, 51) 1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pbmm$ ($Pmma$, 51) 1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pban$ (50) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [2] $Pmmm$ (47) 1; 2; 3; 4; 5; 6; 7; 8
- IIb** [2] $Cccm$ ($\mathbf{c}' = 2\mathbf{c}$) (66); [2] $Ccmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Cmcm$, 63); [2] $Cmcm$ ($\mathbf{c}' = 2\mathbf{c}$) (63); [2] $Ibmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Imma$, 74);
 [2] $Imam$ ($\mathbf{c}' = 2\mathbf{c}$) ($Imma$, 74); [2] $Ibam$ ($\mathbf{c}' = 2\mathbf{c}$) (72); [2] $Immm$ ($\mathbf{c}' = 2\mathbf{c}$) (71)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $Cmmm$ ($\mathbf{c}' = 2\mathbf{c}$) (65); [3] $Cmmm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (65)

Minimal non-isomorphic supergroups

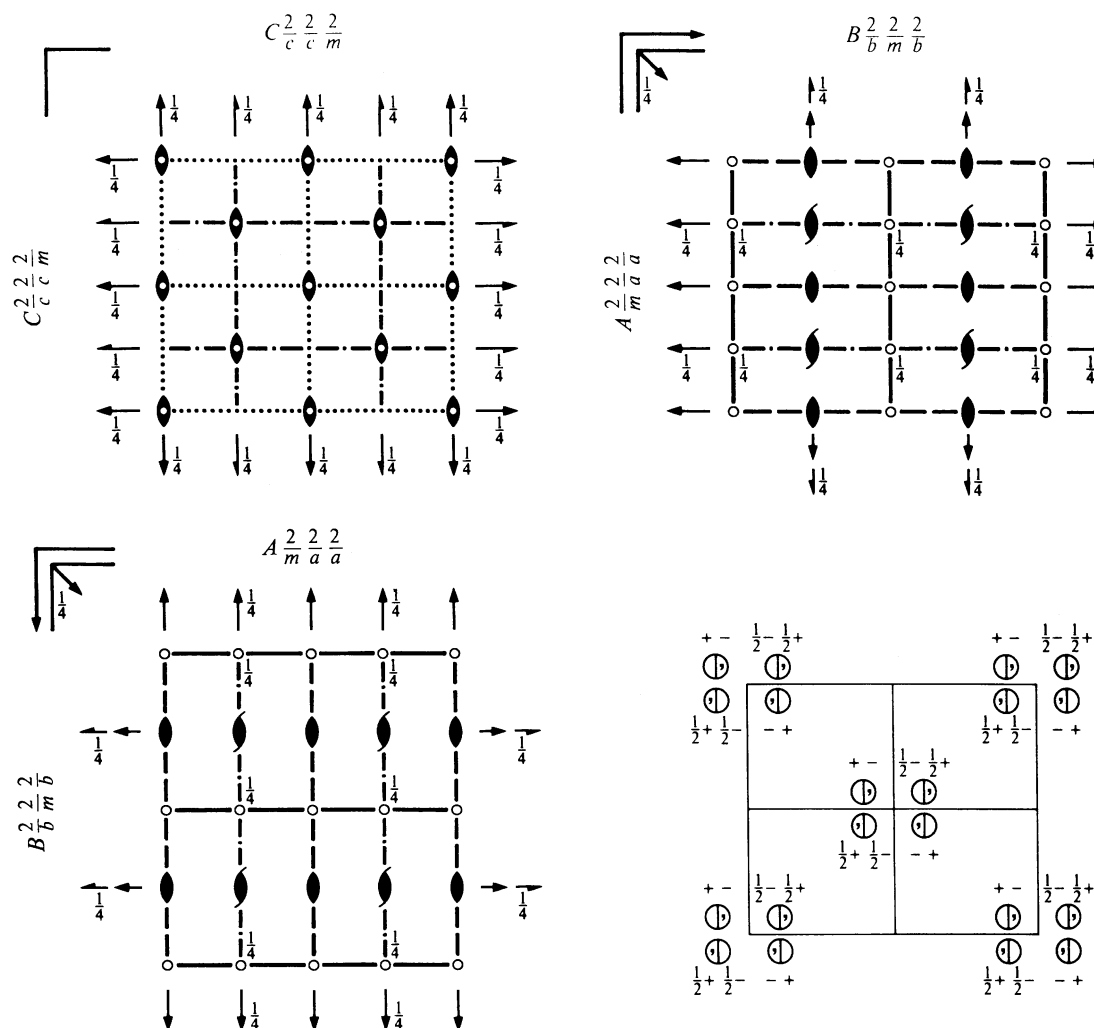
- I** [2] $P4/mmm$ (123); [2] $P4/mbm$ (127); [2] $P4_2/mcm$ (132); [2] $P4_2/mnm$ (136); [3] $P6/mmm$ (191)
- II** [2] $Fmmm$ (69); [2] $Pmmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (47)

$Cccm$
 D_{2h}^{20}
 mmm

Orthorhombic

No. 66

 $C 2/c 2/c 2/m$

 Patterson symmetry $Cmmm$

Origin at centre ($2/m$) at $cc2/m$
Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$
Symmetry operations

 For $(0, 0, 0)+$ set

- | | | | |
|-------------------------|-------------------|-----------------------------|-----------------------------|
| (1) 1 | (2) $2 \ 0, 0, z$ | (3) $2 \ 0, y, \frac{1}{4}$ | (4) $2 \ x, 0, \frac{1}{4}$ |
| (5) $\bar{1} \ 0, 0, 0$ | (6) $m \ x, y, 0$ | (7) $c \ x, 0, z$ | (8) $c \ 0, y, z$ |

 For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 \ \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, 0$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2}) \ x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) \ \frac{1}{4}, y, z$ |

Maximal isomorphic subgroups of lowest index
Ic [3] $Cccm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (66); [3] $Cccm$ ($\mathbf{c}' = 3\mathbf{c}$) (66)

Minimal non-isomorphic supergroups
I [2] $P4/mcc$ (124); [2] $P4/mnc$ (128); [2] $P4_2/mmc$ (131); [2] $P4_2/mbc$ (135); [3] $P6/mcc$ (192)

II [2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (49); [2] $Cmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (65)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
16	<i>m</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) \bar{x},\bar{y},z (6) x,y,\bar{z}	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	$hkl : h+k=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8	<i>l</i> .. <i>m</i>	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	<i>k</i> .. 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$hkl : k+l=2n$
8	<i>j</i> .. 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	$hkl : l=2n$
8	<i>i</i> .. 2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$hkl : l=2n$
8	<i>h</i> . 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	$hkl : l=2n$
8	<i>g</i> 2 ..	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$hkl : l=2n$
4	<i>f</i> .. $2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			$hkl : k+l=2n$
4	<i>e</i> .. $2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : k+l=2n$
4	<i>d</i> .. $2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : l=2n$
4	<i>c</i> .. $2/m$	$0,0,0$	$0,0,\frac{1}{2}$			$hkl : l=2n$
4	<i>b</i> 2 2 2	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			$hkl : l=2n$
4	<i>a</i> 2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			$hkl : l=2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0,0,z$

Along [100] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x,0,0$

Along [010] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Cc2m$ (<i>Ama</i> 2, 40)	(1; 3; 6; 8)+	IIa	[2] $Pnmm$ (58)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C2cm$ (<i>Ama</i> 2, 40)	(1; 4; 6; 7)+		[2] $Pccn$ (56)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $Ccc2$ (37)	(1; 2; 7; 8)+		[2] $Pcnc$ (<i>Pmna</i> , 53)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C222$ (21)	(1; 2; 3; 4)+		[2] $Pncm$ (<i>Pmna</i> , 53)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+		[2] $Pncn$ (<i>Pnna</i> , 52)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C2/c11$ ($C2/c$, 15)	(1; 4; 5; 8)+		[2] $Pcnn$ (<i>Pnna</i> , 52)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[2] $C112/m$ ($P2/m$, 10)	(1; 2; 5; 6)+		[2] $Pccm$ (49)	1; 2; 3; 4; 5; 6; 7; 8
			[2] $Pnnn$ (48)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
			IIb	none	

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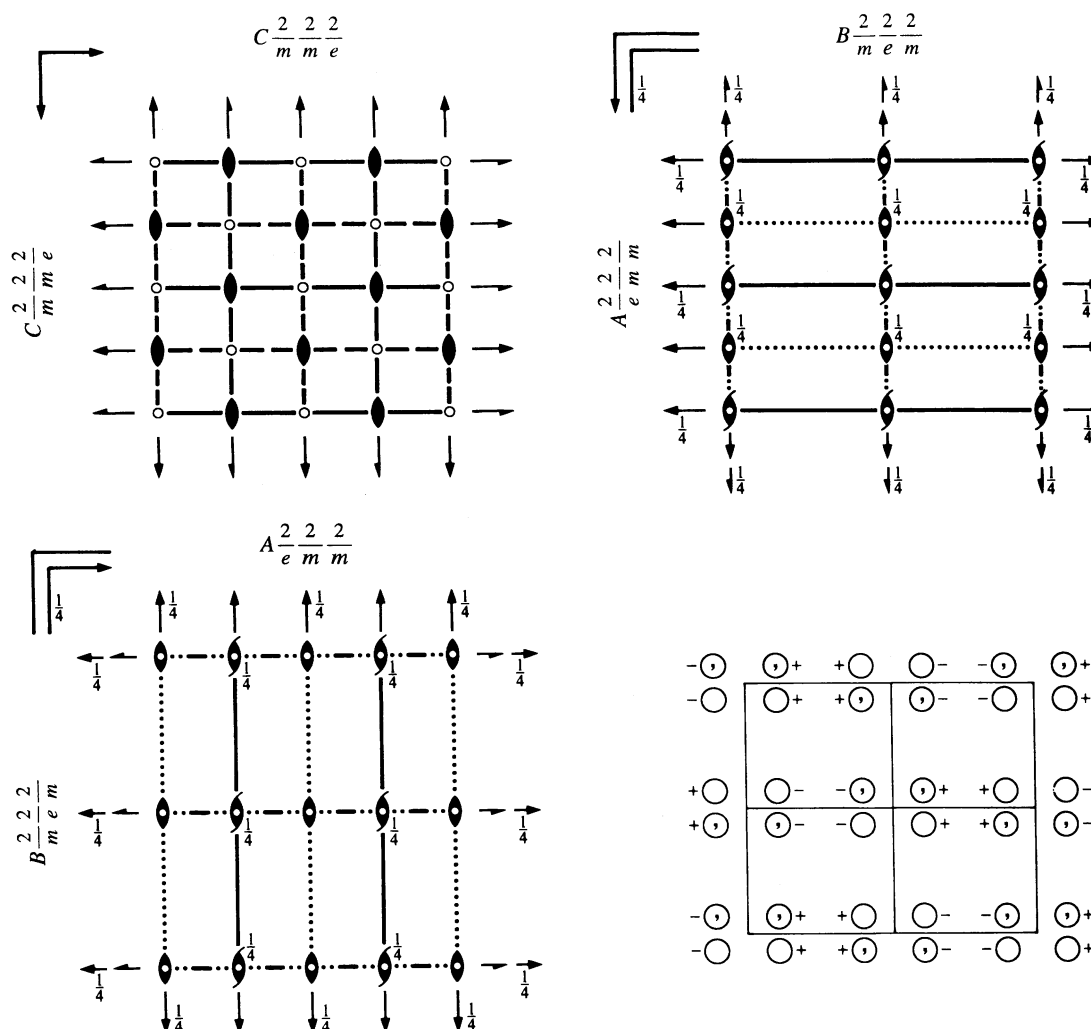
$Cmme$
 D_{2h}^{21}
 mmm

Orthorhombic

No. 67

 $C 2/m 2/m 2/e$

 Patterson symmetry $Cmmm$

 Former space-group symbol $Cmma$; cf. Chapter 1.3

Origin at centre ($2/m$) at $2/m2_1/e$
Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$
Symmetry operations

 For $(0,0,0)+$ set

- | | | | |
|-----------------------------|---------------------------------|--|-----------------------|
| (1) 1 | (2) $2 \quad 0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, 0$ | (4) $2 \quad x, 0, 0$ |
| (5) $\bar{1} \quad 0, 0, 0$ | (6) $b \quad x, y, 0$ | (7) $m \quad x, \frac{1}{4}, z$ | (8) $m \quad 0, y, z$ |

 For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|---------------------------------|---------------------------------|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 \quad \frac{1}{4}, 0, z$ | (3) $2 \quad \frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ |
| (5) $\bar{1} \quad \frac{1}{4}, \frac{1}{4}, 0$ | (6) $a \quad x, y, 0$ | (7) $a \quad x, 0, z$ | (8) $b \quad \frac{1}{4}, y, z$ |

Maximal isomorphic subgroups of lowest index
IIc $[2] Cmme (c' = 2c) (67); [3] Cmme (a' = 3a \text{ or } b' = 3b) (67)$
Minimal non-isomorphic supergroups
I $[2] P4/nbm (125); [2] P4/nmm (129); [2] P4_2/nmm (134); [2] P4_2/nm (138)$
II $[2] Fmmm (69); [2] Pmmm (a' = \frac{1}{2}a, b' = \frac{1}{2}b) (47)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+ $(\frac{1}{2},\frac{1}{2},0)+$				General:
16 o 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) x,\bar{y},\bar{z} (8) \bar{x},y,z	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ Special: as above, plus
8 n .m.	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$	no extra conditions
8 m m..	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8 l ..2	$\frac{1}{4},0,z$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},\frac{1}{2},z$	$hkl : h=2n$
8 k .2.	$\frac{1}{4},y,\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{2}$	$hkl : h=2n$
8 j .2.	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{1}{4},y+\frac{1}{2},0$	$hkl : h=2n$
8 i 2..	$x,0,\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$x,\frac{1}{2},\frac{1}{2}$	$hkl : h=2n$
8 h 2..	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$	$hkl : h=2n$
4 g mm2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4 f .2/m.	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : h=2n$
4 e .2/m.	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			$hkl : h=2n$
4 d 2/m..	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : h=2n$
4 c 2/m..	$0,0,0$	$0,\frac{1}{2},0$			$hkl : h=2n$
4 b 222	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$			$hkl : h=2n$
4 a 222	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$			$hkl : h=2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0,0,z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at x,0,0

Along [010] $p2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] $Cm2e$ ($Aem2$, 39)	(1; 3; 6; 8)+	IIa	[2] $Pbma$ ($Pbcm$, 57)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C2me$ ($Aem2$, 39)	(1; 4; 6; 7)+		[2] $Pmab$ ($Pbcm$, 57)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Cmm2$ (35)	(1; 2; 7; 8)+		[2] $Pbaa$ ($Pcca$, 54)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C222$ (21)	(1; 2; 3; 4)+		[2] $Pbab$ ($Pcca$, 54)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C112/e$ ($P2/c$, 13)	(1; 2; 5; 6)+		[2] $Pmmb$ ($Pmma$, 51)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $C12/m1$ ($C2/m$, 12)	(1; 3; 5; 7)+		[2] $Pmma$ (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+		[2] $Pmaa$ ($Pccm$, 49)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
				[2] $Pbmb$ ($Pccm$, 49)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	[2] $Ccce$ ($\mathbf{c}' = 2\mathbf{c}$) (68); [2] $Ccme$ ($\mathbf{c}' = 2\mathbf{c}$) ($Cmce$, 64); [2] $Cmce$ ($\mathbf{c}' = 2\mathbf{c}$) (64); [2] $Imma$ ($\mathbf{c}' = 2\mathbf{c}$) (74); [2] $Ibca$ ($\mathbf{c}' = 2\mathbf{c}$) (73); [2] $Ibmb$ ($\mathbf{c}' = 2\mathbf{c}$) ($Ibam$, 72); [2] $Imaa$ ($\mathbf{c}' = 2\mathbf{c}$) ($Ibam$, 72)				

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$Ccce$

D_{2h}^{22}

mmm

Orthorhombic

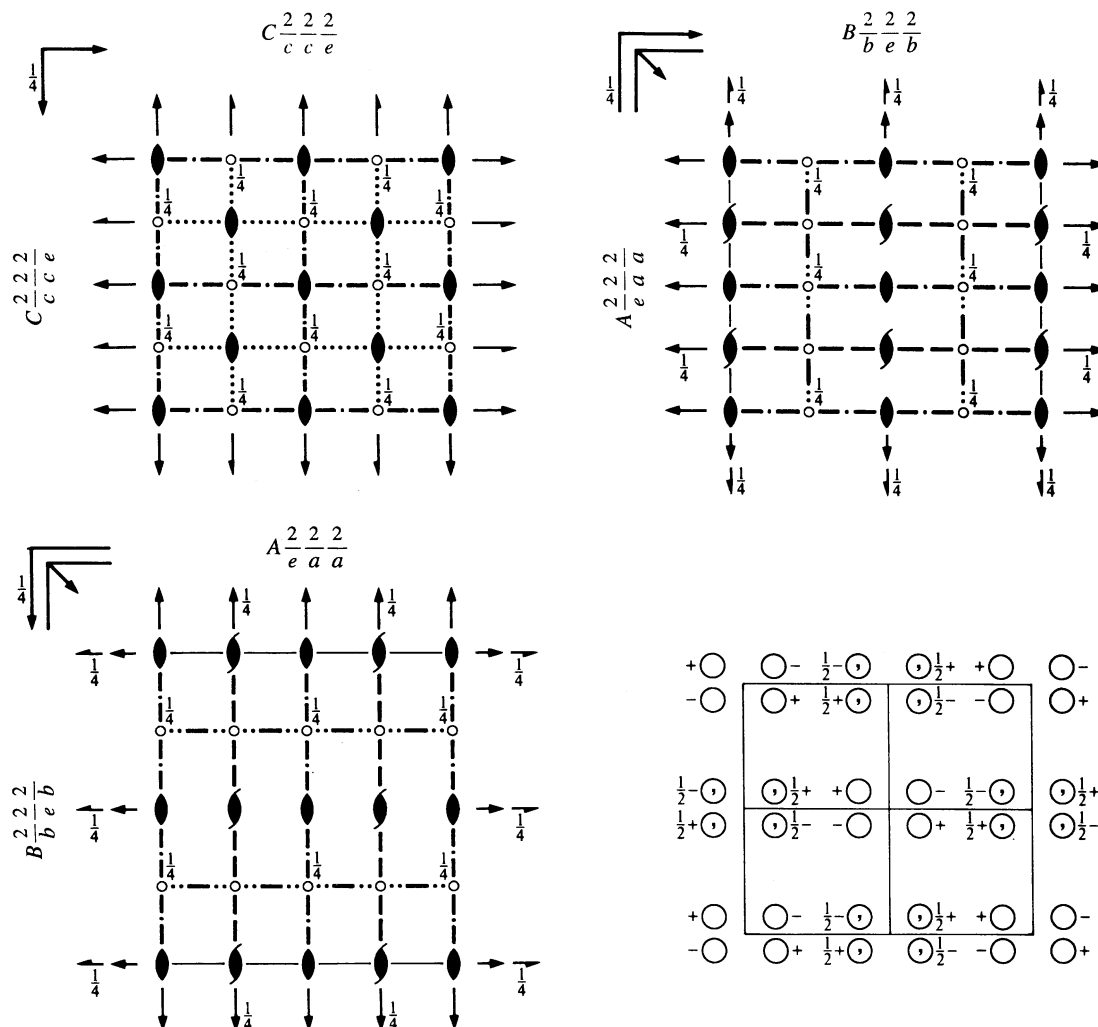
No. 68

$C 2/c 2/c 2/e$

Patterson symmetry $Cmmm$

Former space-group symbol $Ccca$; cf. Chapter 1.3

ORIGIN CHOICE 1



Origin at 222 at $2/n2/n2$, at $0, \frac{1}{4}, \frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---|-------------------------------------|---------------------------|--|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $2 0, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{4}, 0$ |
| (5) $\bar{1} 0, \frac{1}{4}, \frac{1}{4}$ | (6) $a x, y, \frac{1}{4}$ | (7) $c x, \frac{1}{4}, z$ | (8) $c \frac{1}{4}, y, z$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|---------------------------|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 0, 0, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{1}{4}, y, 0$ | (4) $2 x, 0, 0$ |
| (5) $\bar{1} \frac{1}{4}, 0, \frac{1}{4}$ | (6) $b x, y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2}) x, 0, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ |

Generators selected $(1); t(1,0,0); t(0,1,0); t(0,0,1); t(\frac{1}{2},\frac{1}{2},0); (2); (3); (5)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$	General:
16 <i>i</i> 1	(1) x,y,z (5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl : h+k=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	Special: as above, plus
	(3) \bar{x},y,\bar{z} (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$hkl : l=2n$
	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$hkl : k+l=2n$
8 <i>h</i> ..2	$\frac{1}{4},\frac{1}{4},z$ $\frac{3}{4},\frac{1}{4},\bar{z}$ $\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$ $\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$hkl : k+l=2n$
8 <i>g</i> ..2	$0,0,z$ $0,0,\bar{z}$ $0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\frac{1}{2},z+\frac{1}{2}$	$hkl : k+l=2n$
8 <i>f</i> .2.	$0,y,0$ $\frac{1}{2},\bar{y}+\frac{1}{2},0$ $0,\bar{y}+\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},y,\frac{1}{2}$	$hkl : k+l=2n$
8 <i>e</i> 2..	$x,0,0$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$ $\bar{x},\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},0,\frac{1}{2}$	$hkl : k+l=2n$
8 <i>d</i> $\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$ $\frac{1}{2},\frac{1}{4},\frac{1}{4}$ $0,\frac{1}{4},\frac{3}{4}$ $\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$hkl : k,l=2n$
8 <i>c</i> $\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$ $\frac{1}{4},\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},0,\frac{3}{4}$ $\frac{3}{4},\frac{1}{2},\frac{3}{4}$	$hkl : k,l=2n$
4 <i>b</i> 222	$0,0,\frac{1}{2}$ $0,\frac{1}{2},0$	$hkl : k+l=2n$
4 <i>a</i> 222	$0,0,0$ $0,\frac{1}{2},\frac{1}{2}$	$hkl : k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Cc2e$ ($Aea2, 41$)	$(1; 3; 6; 8)+$
	[2] $C2ce$ ($Aea2, 41$)	$(1; 4; 6; 7)+$
	[2] $Ccc2$ (37)	$(1; 2; 7; 8)+$
	[2] $C222$ (21)	$(1; 2; 3; 4)+$
	[2] $C12/c1$ ($C2/c, 15$)	$(1; 3; 5; 7)+$
	[2] $C2/c11$ ($C2/c, 15$)	$(1; 4; 5; 8)+$
	[2] $C112/e$ ($P2/c, 13$)	$(1; 2; 5; 6)+$
IIa	[2] $Pcnb$ ($Pbcn, 60$)	$1; 4; 5; 8; (2; 3; 6; 7) + (\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnca$ ($Pbcn, 60$)	$1; 4; 6; 7; (2; 3; 5; 8) + (\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcca$ (54)	$1; 2; 3; 4; 5; 6; 7; 8$
	[2] $Pccb$ ($Pcca, 54$)	$1; 2; 7; 8; (3; 4; 5; 6) + (\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnnb$ ($Pnna, 52$)	$1; 2; 3; 4; (5; 6; 7; 8) + (\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnna$ (52)	$1; 2; 5; 6; (3; 4; 7; 8) + (\frac{1}{2},\frac{1}{2},0)$
	[2] $Pncb$ ($Pban, 50$)	$1; 3; 5; 7; (2; 4; 6; 8) + (\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcna$ ($Pban, 50$)	$1; 3; 6; 8; (2; 4; 5; 7) + (\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ccce$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (68); [3] $Ccce$ ($\mathbf{c}' = 3\mathbf{c}$) (68)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)
II [2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (49); [2] $Cmme$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)

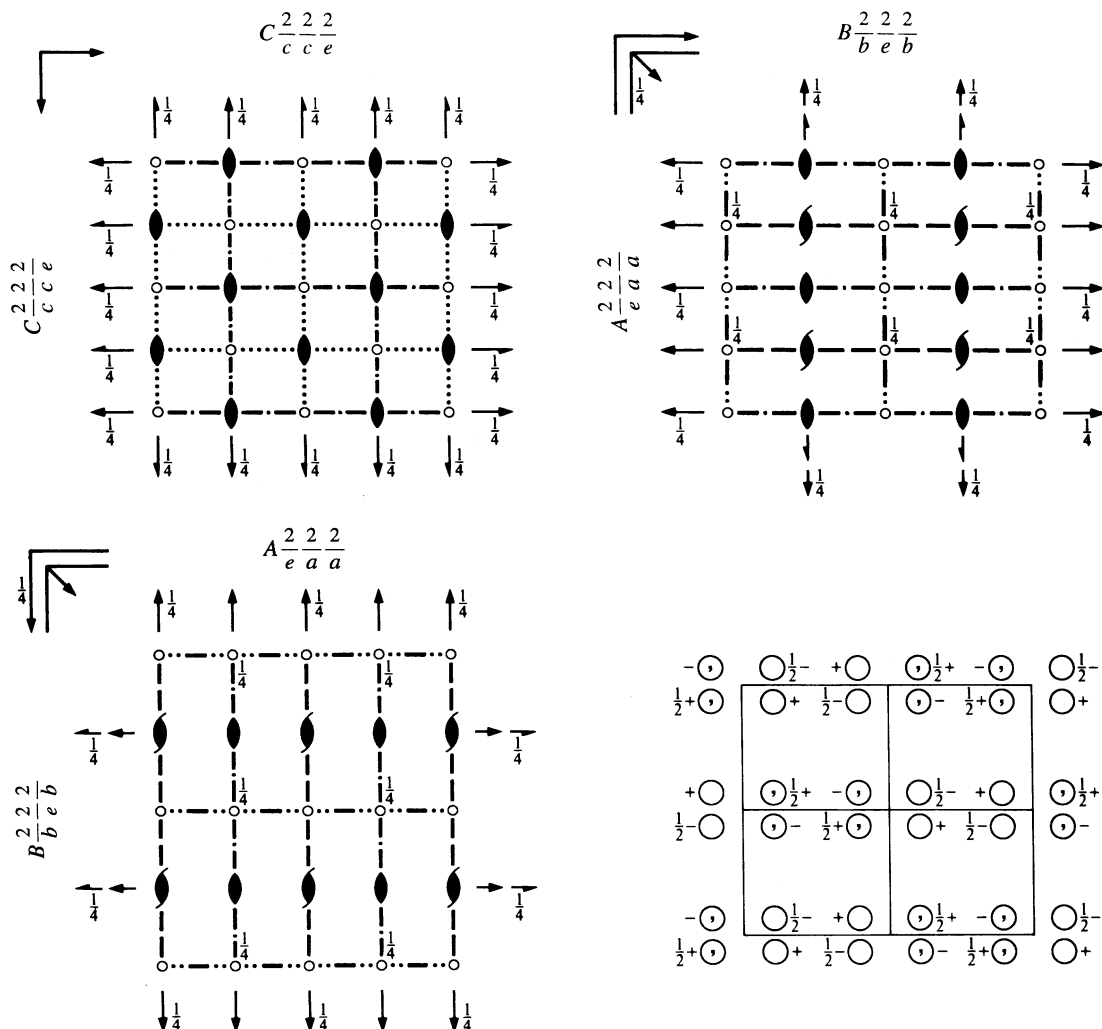
$Ccce$ D_{2h}^{22} mmm

Orthorhombic

No. 68

 $C 2/c 2/c 2/e$ Patterson symmetry $Cmmm$ Former space-group symbol $Ccca$; cf. Chapter 1.3

ORIGIN CHOICE 2

Origin at $\bar{1}$ at nce , at $0, -\frac{1}{4}, -\frac{1}{4}$ from 222Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$ **Symmetry operations**For $(0,0,0)+$ set

- | | | | |
|-----------------------|---------------------------|---------------------------|--|
| (1) 1 | (2) $2 \frac{1}{4}, 0, z$ | (3) $2 0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{4}$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $a x, y, 0$ | (7) $c x, 0, z$ | (8) $c \frac{1}{4}, y, z$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|---------------------------|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{1}{4}, y, \frac{1}{4}$ | (4) $2 x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1} \frac{1}{4}, \frac{1}{4}, 0$ | (6) $b x, y, 0$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2}) x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$	General:
16 <i>i</i> 1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (5) \bar{x},\bar{y},\bar{z} (6) $x+\frac{1}{2},y,\bar{z}$ (7) $x,\bar{y},z+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$hkl : h+k=2n$ $Ok_l : k,l=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8 <i>h</i> ..2	$\frac{1}{4},0,z$ $\frac{3}{4},0,\bar{z}+\frac{1}{2}$ $\frac{3}{4},0,\bar{z}$ $\frac{1}{4},0,z+\frac{1}{2}$	$hkl : l=2n$
8 <i>g</i> ..2	$0,\frac{1}{4},z$ $0,\frac{1}{4},\bar{z}+\frac{1}{2}$ $0,\frac{3}{4},\bar{z}$ $0,\frac{3}{4},z+\frac{1}{2}$	$hkl : k+l=2n$
8 <i>f</i> .2.	$0,y,\frac{1}{4}$ $\frac{1}{2},\bar{y},\frac{1}{4}$ $0,\bar{y},\frac{3}{4}$ $\frac{1}{2},y,\frac{3}{4}$	$hkl : k+l=2n$
8 <i>e</i> 2..	$x,\frac{1}{4},\frac{1}{4}$ $\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$ $\bar{x},\frac{3}{4},\frac{3}{4}$ $x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$hkl : k+l=2n$
8 <i>d</i> $\bar{1}$	$0,0,0$ $\frac{1}{2},0,0$ $0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$	$hkl : k,l=2n$
8 <i>c</i> $\bar{1}$	$\frac{1}{4},\frac{3}{4},0$ $\frac{1}{4},\frac{1}{4},0$ $\frac{3}{4},\frac{3}{4},\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$hkl : k,l=2n$
4 <i>b</i> 222	$0,\frac{1}{4},\frac{3}{4}$ $0,\frac{3}{4},\frac{1}{4}$	$hkl : k+l=2n$
4 <i>a</i> 222	$0,\frac{1}{4},\frac{1}{4}$ $0,\frac{3}{4},\frac{3}{4}$	$hkl : k+l=2n$
Symmetry of special projections		
Along [001] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ Origin at 0,0,z	Along [100] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at x,0,0	Along [010] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$ Origin at 0,y,0
Maximal non-isomorphic subgroups		
I	[2] $Cc2e$ ($Aea2, 41$) (1; 3; 6; 8)+ [2] $C2ce$ ($Aea2, 41$) (1; 4; 6; 7)+ [2] $Ccc2$ (37) (1; 2; 7; 8)+ [2] $C222$ (21) (1; 2; 3; 4)+ [2] $C12/c1$ ($C2/c, 15$) (1; 3; 5; 7)+ [2] $C2/c11$ ($C2/c, 15$) (1; 4; 5; 8)+ [2] $C112/e$ ($P2/c, 13$) (1; 2; 5; 6)+	
IIa	[2] $Pcnb$ ($Pbcn, 60$) 1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $Pnca$ ($Pbcn, 60$) 1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $Pcca$ (54) 1; 2; 3; 4; 5; 6; 7; 8 [2] $Pccb$ ($Pcca, 54$) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $Pnnb$ ($Pnna, 52$) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $Pnna$ (52) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $Pncb$ ($Pban, 50$) 1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$ [2] $Pcna$ ($Pban, 50$) 1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	
IIb	none	
Maximal isomorphic subgroups of lowest index		
IIc	[3] $Ccce$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (68); [3] $Ccce$ ($\mathbf{c}' = 3\mathbf{c}$) (68)	
Minimal non-isomorphic supergroups		
I	[2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)	
II	[2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (49); [2] $Cmme$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)	

$F m m m$

D_{2h}^{23}

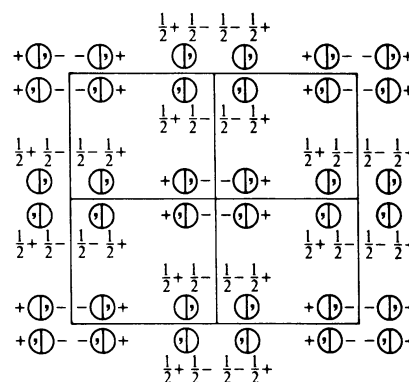
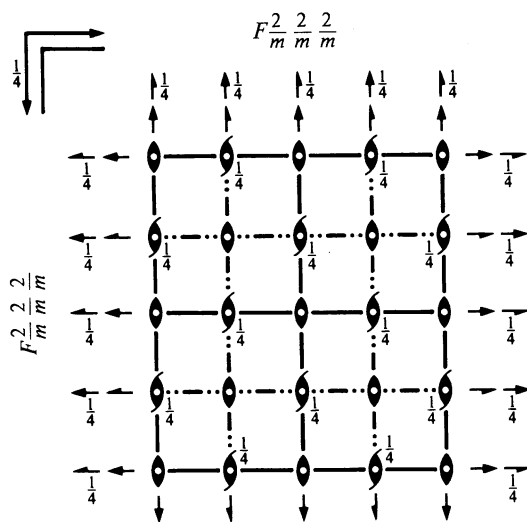
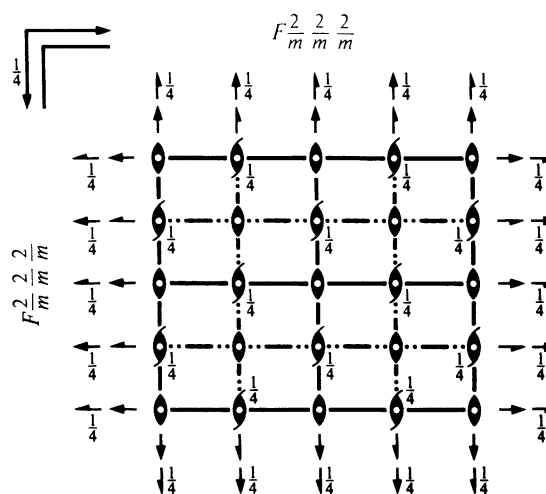
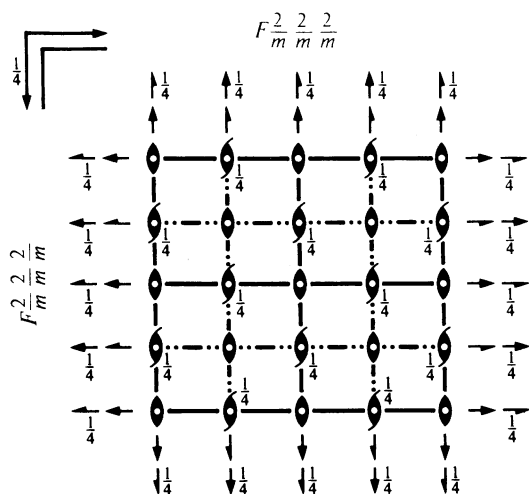
$m m m$

Orthorhombic

No. 69

$F 2/m 2/m 2/m$

Patterson symmetry $F m m m$



Origin at centre (mmm)

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------------|-----------------|-----------------|-----------------|
| (1) $\bar{1}$ | (2) $2 \ 0,0,z$ | (3) $2 \ 0,y,0$ | (4) $2 \ x,0,0$ |
| (5) $\bar{1} \ 0,0,0$ | (6) $m \ x,y,0$ | (7) $m \ x,0,z$ | (8) $m \ 0,y,z$ |

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--|---|---|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0, \frac{1}{2}) \ 0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \ 0,y, \frac{1}{4}$ | (4) $2 \ x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1} \ 0, \frac{1}{4}, \frac{1}{4}$ | (6) $b \ x,y, \frac{1}{4}$ | (7) $c \ x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) \ 0,y,z$ |

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- | | | | |
|---|---|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0,0, \frac{1}{2}) \ \frac{1}{4}, 0, z$ | (3) $2 \ \frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \ x, 0, \frac{1}{4}$ |
| (5) $\bar{1} \ \frac{1}{4}, 0, \frac{1}{4}$ | (6) $a \ x,y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2}) \ x, 0, z$ | (8) $c \ \frac{1}{4}, y, z$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 \ \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, 0$ |
| (5) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x,y,0$ | (7) $a \ x, \frac{1}{4}, z$ | (8) $b \ \frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	
32 <i>p</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) \bar{x}, y, \bar{z} (7) x, \bar{y}, z	(4) x, \bar{y}, \bar{z} (8) \bar{x}, y, z	General: $hkl : h+k, h+l, k+l = 2n$ $0kl : k, l = 2n$ $h0l : h, l = 2n$ $hk0 : h, k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
16 <i>o</i> $. . m$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, 0$	$x, \bar{y}, 0$	no extra conditions
16 <i>n</i> $. m .$	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x}, 0, \bar{z}$	$x, 0, \bar{z}$	no extra conditions
16 <i>m</i> $m . .$	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$	no extra conditions
16 <i>l</i> $2 . .$	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x, \frac{1}{4}, \frac{3}{4}$	$hkl : h = 2n$
16 <i>k</i> $. 2 .$	$\frac{1}{4}, y, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, y, \frac{3}{4}$	$hkl : h = 2n$
16 <i>j</i> $. . 2$	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, z$	$hkl : h = 2n$
8 <i>i</i> $m m 2$	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
8 <i>h</i> $m 2 m$	$0, y, 0$	$0, \bar{y}, 0$			no extra conditions
8 <i>g</i> $2 m m$	$x, 0, 0$	$\bar{x}, 0, 0$			no extra conditions
8 <i>f</i> $2 2 2$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h = 2n$
8 <i>e</i> $. . 2/m$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$			$hkl : h = 2n$
8 <i>d</i> $. 2/m .$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{3}{4}, 0, \frac{1}{4}$			$hkl : h = 2n$
8 <i>c</i> $2/m . .$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$			$hkl : h = 2n$
4 <i>b</i> $m m m$	$0, 0, \frac{1}{2}$				no extra conditions
4 <i>a</i> $m m m$	$0, 0, 0$				no extra conditions

Symmetry of special projections

Along $[001]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along $[010]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] <i>F m m 2</i> (42)	(1; 2; 7; 8)+
	[2] <i>F m 2 m</i> (<i>F m m 2</i> , 42)	(1; 3; 6; 8)+
	[2] <i>F 2 m m</i> (<i>F m m 2</i> , 42)	(1; 4; 6; 7)+
	[2] <i>F 2 2 2</i> (22)	(1; 2; 3; 4)+
	[2] <i>F 1 1 2/m</i> (<i>C 2/m</i> , 12)	(1; 2; 5; 6)+
	[2] <i>F 1 2/m 1</i> (<i>C 2/m</i> , 12)	(1; 3; 5; 7)+
	[2] <i>F 2/m 1 1</i> (<i>C 2/m</i> , 12)	(1; 4; 5; 8)+
IIa	[2] <i>A e a a</i> (<i>C c c e</i> , 68)	1; 2; 3; 4; (1; 2; 3; 4) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (5; 6; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (5; 6; 7; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>B b e b</i> (<i>C c c e</i> , 68)	1; 2; 3; 4; (1; 2; 3; 4) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (5; 6; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (5; 6; 7; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>C c c e</i> (68)	1; 2; 3; 4; (1; 2; 3; 4) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (5; 6; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (5; 6; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>C m m e</i> (67)	1; 2; 7; 8; (1; 2; 7; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (3; 4; 5; 6) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>B m e m</i> (<i>C m m e</i> , 67)	1; 3; 6; 8; (1; 3; 6; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 4; 5; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>A e m m</i> (<i>C m m e</i> , 67)	1; 4; 6; 7; (1; 4; 6; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 5; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 3; 5; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>C c c m</i> (66)	1; 2; 5; 6; (1; 2; 5; 6) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (3; 4; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>B b m b</i> (<i>C c c m</i> , 66)	1; 3; 5; 7; (1; 3; 5; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 4; 6; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 6; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>A m a a</i> (<i>C c c m</i> , 66)	1; 4; 5; 8; (1; 4; 5; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 6; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 3; 6; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>A m m m</i> (<i>C m m m</i> , 65)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$)
	[2] <i>B m m m</i> (<i>C m m m</i> , 65)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>C m m m</i> (65)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>A e a m</i> (<i>C m c e</i> , 64)	1; 2; 5; 6; (1; 2; 5; 6) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (3; 4; 7; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>B b e m</i> (<i>C m c e</i> , 64)	1; 2; 5; 6; (1; 2; 5; 6) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (3; 4; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 7; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>A e m a</i> (<i>C m c e</i> , 64)	1; 3; 5; 7; (1; 3; 5; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 6; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 4; 6; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>C c m e</i> (<i>C m c e</i> , 64)	1; 3; 5; 7; (1; 3; 5; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (2; 4; 6; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 6; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>B m e b</i> (<i>C m c e</i> , 64)	1; 4; 5; 8; (1; 4; 5; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 3; 6; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 6; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>C m c e</i> (64)	1; 4; 5; 8; (1; 4; 5; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (2; 3; 6; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 6; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>A m a m</i> (<i>C m c m</i> , 63)	1; 3; 6; 8; (1; 3; 6; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>A m m a</i> (<i>C m c m</i> , 63)	1; 2; 7; 8; (1; 2; 7; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>B m m b</i> (<i>C m c m</i> , 63)	1; 2; 7; 8; (1; 2; 7; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (3; 4; 5; 6) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (3; 4; 5; 6) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>B b m m</i> (<i>C m c m</i> , 63)	1; 4; 6; 7; (1; 4; 6; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$); (2; 3; 5; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 5; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0)
	[2] <i>C m c m</i> (63)	1; 3; 6; 8; (1; 3; 6; 8) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (2; 4; 5; 7) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 4; 5; 7) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)
	[2] <i>C c m m</i> (<i>C m c m</i> , 63)	1; 4; 6; 7; (1; 4; 6; 7) + ($\frac{1}{2}$, $\frac{1}{2}$, 0); (2; 3; 5; 8) + (0, $\frac{1}{2}$, $\frac{1}{2}$); (2; 3; 5; 8) + ($\frac{1}{2}$, 0, $\frac{1}{2}$)

IIIb none

Maximal isomorphic subgroups of lowest index

IIIc [3] *F m m m* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (69)

Minimal non-isomorphic supergroups

I [2] *I 4/m m m* (139); [2] *I 4/m c m* (140); [3] *F m 3* (202)

II [2] *P m m m* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (47)

$F d d d$

D_{2h}^{24}

$m m m$

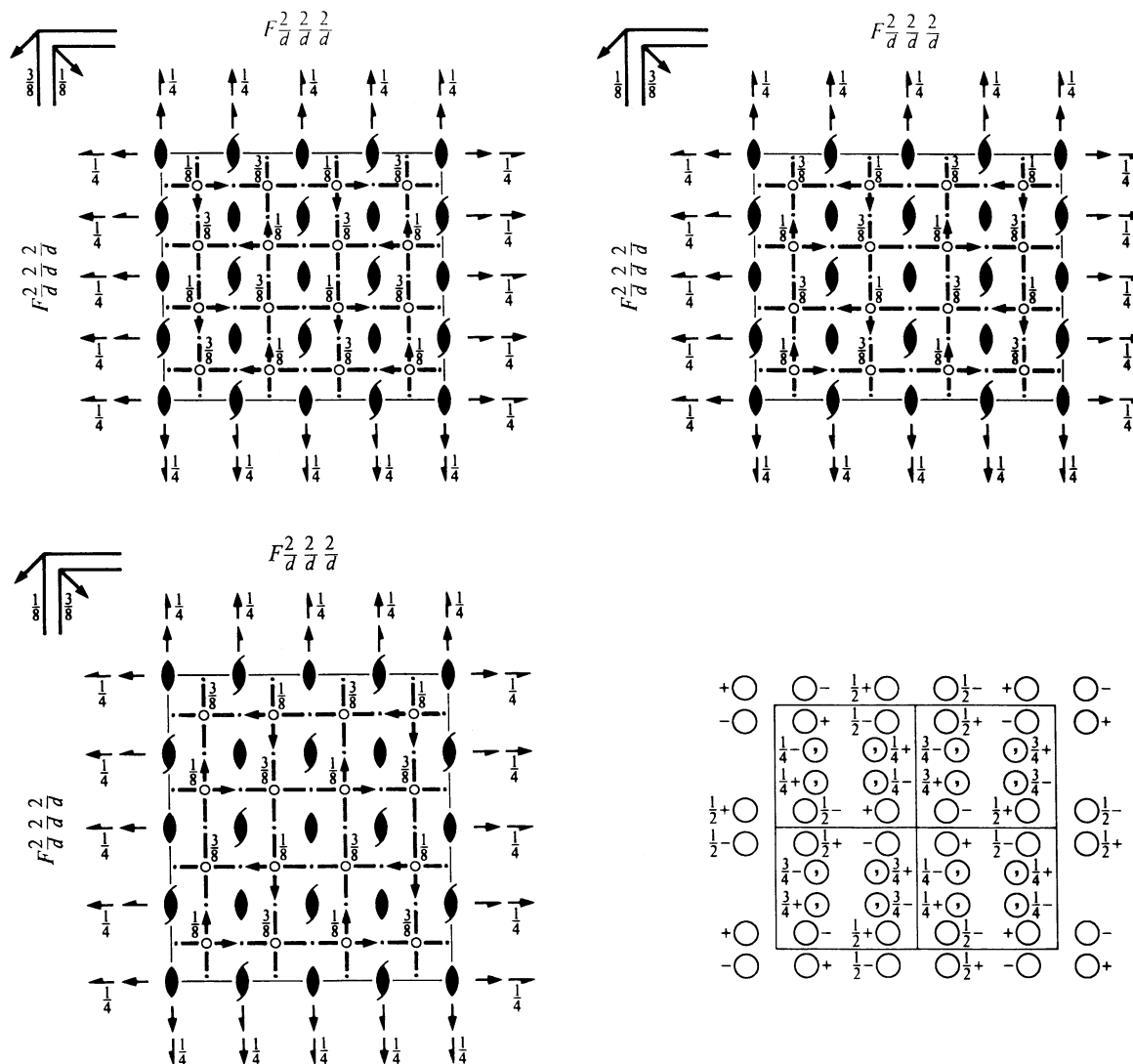
Orthorhombic

No. 70

$F 2/d 2/d 2/d$

Patterson symmetry $F m m m$

ORIGIN CHOICE 1



Origin at 222, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---|--|--|--|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) $\bar{1}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (6) $d(\frac{1}{4}, \frac{1}{4}, 0)$ $x, y, \frac{1}{8}$ | (7) $d(\frac{1}{4}, 0, \frac{1}{4})$ $x, \frac{1}{8}, z$ | (8) $d(0, \frac{1}{4}, \frac{1}{4})$ $\frac{1}{8}, y, z$ |

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|--|--|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $(0, 0, \frac{1}{2})$ $0, \frac{1}{4}, z$ | (3) 2 $(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) 2 $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$ | (6) $d(\frac{1}{4}, \frac{3}{4}, 0)$ $x, y, \frac{3}{8}$ | (7) $d(\frac{1}{4}, 0, \frac{3}{4})$ $x, \frac{3}{8}, z$ | (8) $d(0, \frac{3}{4}, \frac{3}{4})$ $\frac{1}{8}, y, z$ |

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) 2 $(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2 $(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{3}{8}, \frac{1}{8}, \frac{3}{8}$ | (6) $d(\frac{3}{4}, \frac{1}{4}, 0)$ $x, y, \frac{3}{8}$ | (7) $d(\frac{3}{4}, 0, \frac{1}{4})$ $x, \frac{1}{8}, z$ | (8) $d(0, \frac{1}{4}, \frac{3}{4})$ $\frac{3}{8}, y, z$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2 $(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) 2 $(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $\frac{3}{8}, \frac{3}{8}, \frac{1}{8}$ | (6) $d(\frac{3}{4}, \frac{3}{4}, 0)$ $x, y, \frac{1}{8}$ | (7) $d(\frac{3}{4}, 0, \frac{1}{4})$ $x, \frac{3}{8}, z$ | (8) $d(0, \frac{3}{4}, \frac{1}{4})$ $\frac{3}{8}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5)

Positions

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	General:
32	<i>h</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(3) \bar{x}, y, \bar{z} (7) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{1}{4}$	(4) x, \bar{y}, \bar{z} (8) $\bar{x} + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	hkl : $h + k = 2n$ and $h + l, k + l = 2n$ $0kl$: $k + l = 4n$ and $k, l = 2n$ $h0l$: $h + l = 4n$ and $h, l = 2n$ $hk0$: $h + k = 4n$ and $h, k = 2n$ $h00$: $h = 4n$ $0k0$: $k = 4n$ $00l$: $l = 4n$
16	<i>g</i> ..2	0,0, z	0,0, \bar{z}	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{4}$	hkl : $h = 2n + 1$ or $h + k + l = 4n$
16	<i>f</i> .2.	0, y ,0	0, \bar{y} ,0	$\frac{1}{4}, \bar{y} + \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, y + \frac{1}{4}, \frac{1}{4}$	
16	<i>e</i> 2..	x ,0,0	\bar{x} ,0,0	$\bar{x} + \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$x + \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	
16	<i>d</i> $\bar{1}$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{3}{8}$	hkl : $h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$
16	<i>c</i> $\bar{1}$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{7}{8}$	
8	<i>b</i> 222	0,0, $\frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	hkl : $h = 2n + 1$ or $h + k + l = 4n$	
8	<i>a</i> 222	0,0,0	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$			

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0,0, z

Along [100] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at 0, y ,0

Maximal non-isomorphic subgroups

I	[2] $Fdd2$ (43)	(1; 2; 7; 8)+
	[2] $Fd2d$ ($Fdd2$, 43)	(1; 3; 6; 8)+
	[2] $F2dd$ ($Fdd2$, 43)	(1; 4; 6; 7)+
	[2] $F222$ (22)	(1; 2; 3; 4)+
	[2] $F112/d$ ($C2/c$, 15)	(1; 2; 5; 6)+
	[2] $F12/d1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $F2/d11$ ($C2/c$, 15)	(1; 4; 5; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Fddd$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (70)

Minimal non-isomorphic supergroups

I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)

II [2] $Pnnn$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (48)

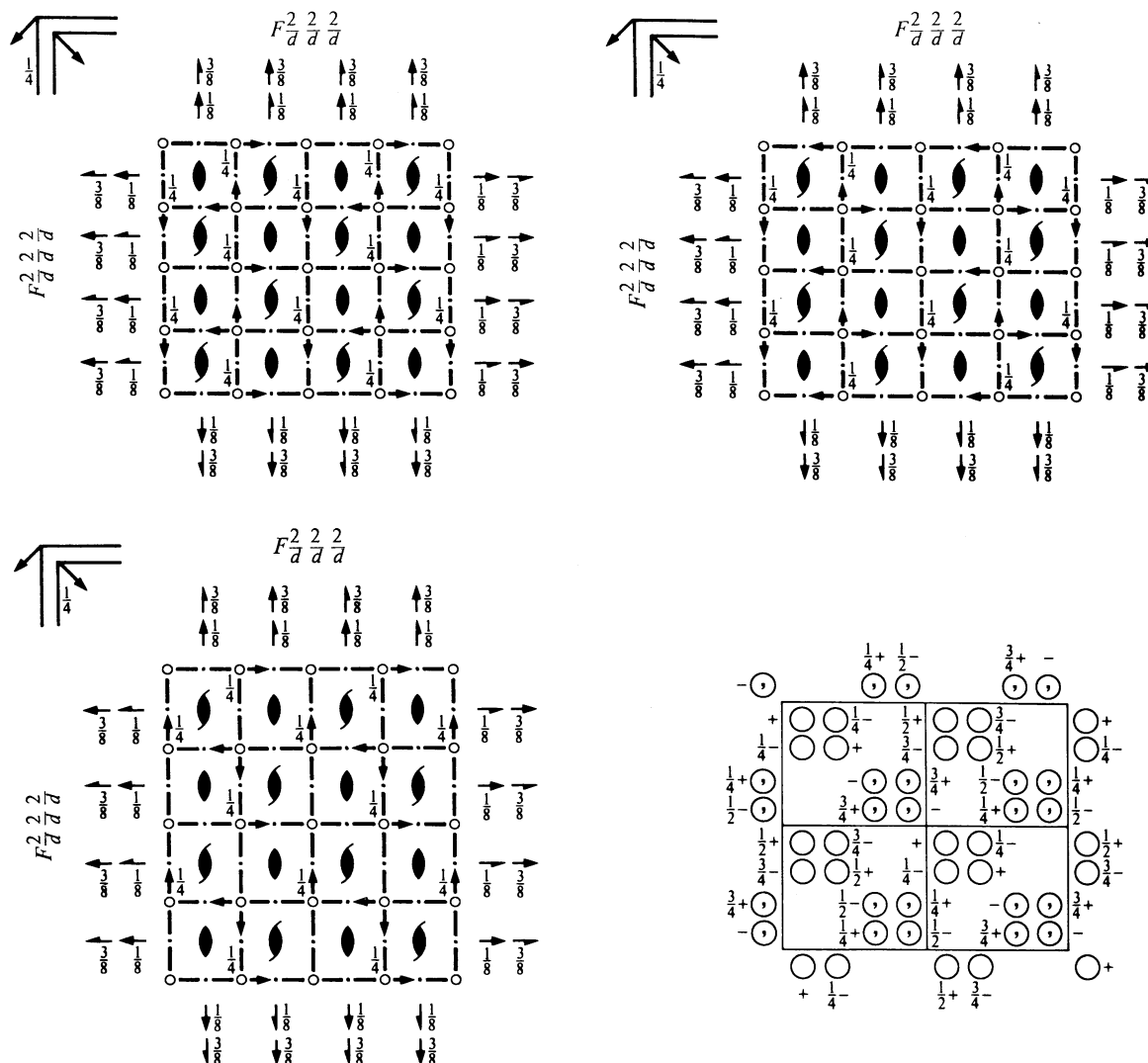
$F d d d$ D_{2h}^{24} $m m m$

Orthorhombic

No. 70

 $F 2/d 2/d 2/d$ Patterson symmetry $F m m m$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $d d d$, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 222Asymmetric unit $0 \leq x \leq \frac{1}{8}$; $-\frac{1}{8} \leq y \leq \frac{1}{8}$; $0 \leq z \leq 1$ **Symmetry operations**For $(0, 0, 0)+$ set

- | | | | |
|-----------------------|--|--|--|
| (1) 1 | (2) $2 \frac{1}{8}, \frac{3}{8}, z$ | (3) $2 \frac{3}{8}, y, \frac{3}{8}$ | (4) $2 x, \frac{3}{8}, \frac{3}{8}$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $d(\frac{1}{4}, \frac{1}{4}, 0) x, y, 0$ | (7) $d(\frac{1}{4}, 0, \frac{1}{4}) x, 0, z$ | (8) $d(0, \frac{1}{4}, \frac{1}{4}) 0, y, z$ |

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|--|--|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \frac{3}{8}, \frac{1}{8}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{3}{8}, y, \frac{1}{8}$ | (4) $2 x, \frac{1}{8}, \frac{1}{8}$ |
| (5) $\bar{1} 0, \frac{1}{4}, \frac{1}{4}$ | (6) $d(\frac{1}{4}, \frac{3}{4}, 0) x, y, \frac{1}{4}$ | (7) $d(\frac{1}{4}, 0, \frac{3}{4}) x, \frac{1}{4}, z$ | (8) $d(0, \frac{3}{4}, \frac{3}{4}) 0, y, z$ |

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \frac{1}{8}, \frac{3}{8}, z$ | (3) $2 \frac{1}{8}, y, \frac{1}{8}$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{3}{8}, \frac{1}{8}$ |
| (5) $\bar{1} \frac{1}{4}, 0, \frac{1}{4}$ | (6) $d(\frac{3}{4}, \frac{1}{4}, 0) x, y, \frac{1}{4}$ | (7) $d(\frac{3}{4}, 0, \frac{3}{4}) x, 0, z$ | (8) $d(0, \frac{1}{4}, \frac{3}{4}) \frac{1}{4}, y, z$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 \frac{1}{8}, \frac{1}{8}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{1}{8}, y, \frac{3}{8}$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{8}, \frac{3}{8}$ |
| (5) $\bar{1} \frac{1}{4}, \frac{1}{4}, 0$ | (6) $d(\frac{3}{4}, \frac{3}{4}, 0) x, y, 0$ | (7) $d(\frac{3}{4}, 0, \frac{1}{4}) x, \frac{1}{4}, z$ | (8) $d(0, \frac{3}{4}, \frac{1}{4}) \frac{1}{4}, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	General:
32	<i>h</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, z$ (6) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z}$	(3) $\bar{x} + \frac{3}{4}, y, \bar{z} + \frac{3}{4}$ (7) $x + \frac{1}{4}, \bar{y}, z + \frac{1}{4}$	(4) $x, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (8) $\bar{x}, y + \frac{1}{4}, z + \frac{1}{4}$	$hkl : h+k, h+l, k+l = 2n$ $Ok l : k+l = 4n, k, l = 2n$ $hOl : h+l = 4n, h, l = 2n$ $hk0 : h+k = 4n, h, k = 2n$ $h00 : h = 4n$ $Ok0 : k = 4n$ $00l : l = 4n$
16	<i>g</i> ..2	$\frac{1}{8}, \frac{1}{8}, z$	$\frac{5}{8}, \frac{1}{8}, \bar{z} + \frac{3}{4}$	$\frac{7}{8}, \frac{7}{8}, \bar{z}$	$\frac{3}{8}, \frac{7}{8}, z + \frac{1}{4}$	$hkl : h = 2n + 1$ or $h+k+l = 4n$
16	<i>f</i> .2.	$\frac{1}{8}, y, \frac{1}{8}$	$\frac{5}{8}, \bar{y} + \frac{3}{4}, \frac{1}{8}$	$\frac{7}{8}, \bar{y}, \frac{7}{8}$	$\frac{3}{8}, y + \frac{1}{4}, \frac{7}{8}$	
16	<i>e</i> 2..	$x, \frac{1}{8}, \frac{1}{8}$	$\bar{x} + \frac{3}{4}, \frac{5}{8}, \frac{1}{8}$	$\bar{x}, \frac{7}{8}, \frac{7}{8}$	$x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}$	
16	<i>d</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$
16	<i>c</i> $\bar{1}$	0,0,0	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{3}{4}$	$0, \frac{3}{4}, \frac{3}{4}$	
8	<i>b</i> 222	$\frac{1}{8}, \frac{1}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{3}{8}$			$hkl : h = 2n + 1$ or $h+k+l = 4n$
8	<i>a</i> 222	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$			

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{8}, \frac{1}{8}, z$

Along [100] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, \frac{1}{8}, \frac{1}{8}$

Along [010] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $\frac{1}{8}, y, \frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $Fddd(43)$	(1; 2; 7; 8)+
	[2] $Fd2d(Fdd2, 43)$	(1; 3; 6; 8)+
	[2] $F2dd(Fdd2, 43)$	(1; 4; 6; 7)+
	[2] $F222(22)$	(1; 2; 3; 4)+
	[2] $F112/d(C2/c, 15)$	(1; 2; 5; 6)+
	[2] $F12/d1(C2/c, 15)$	(1; 3; 5; 7)+
	[2] $F2/d11(C2/c, 15)$	(1; 4; 5; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Fddd(\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c})(70)$

Minimal non-isomorphic supergroups

I [2] $I4_1/amd(141)$; [2] $I4_1/acd(142)$; [3] $Fd\bar{3}(203)$

II [2] $Pnnn(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})(48)$

$I m m m$

D_{2h}^{25}

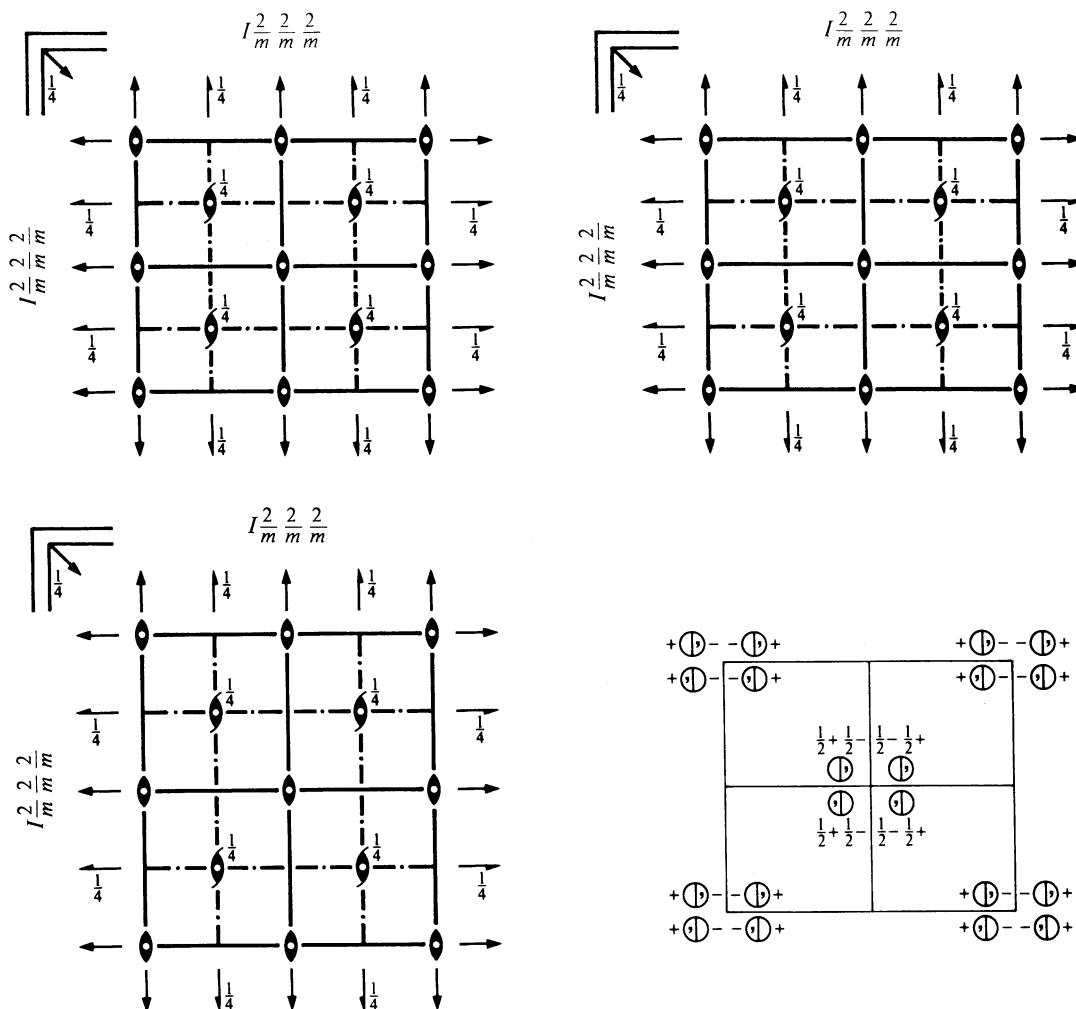
$m m m$

Orthorhombic

No. 71

$I 2/m 2/m 2/m$

Patterson symmetry $I m m m$



Origin at centre ($m m m$)

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------------|-----------------|-----------------|-----------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) m $x,y,0$ | (7) m $x,0,z$ | (8) m $0,y,z$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |

Maximal isomorphic subgroups of lowest index

IIc [3] $I m m m$ ($a' = 3a$ or $b' = 3b$ or $c' = 3c$) (71)

Minimal non-isomorphic supergroups

I [2] $I 4/m m m$ (139); [3] $I m \bar{3}$ (204)

II [2] $A m m m$ ($a' = \frac{1}{2}a$) ($C m m m$, 65); [2] $B m m m$ ($b' = \frac{1}{2}b$) ($C m m m$, 65); [2] $C m m m$ ($c' = \frac{1}{2}c$) (65)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16 <i>o</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) \bar{x}, y, \bar{z} (7) x, \bar{y}, z	(4) x, \bar{y}, \bar{z} (8) \bar{x}, y, z	$hkl : h+k+l=2n$ $Ok\bar{l} : k+l=2n$ $h0l : h+l=2n$ $hk0 : h+k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$ Special: as above, plus
8 <i>n</i> . . <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, 0$	$x, \bar{y}, 0$	no extra conditions
8 <i>m</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x}, 0, \bar{z}$	$x, 0, \bar{z}$	no extra conditions
8 <i>l</i> <i>m</i> . .	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$	no extra conditions
8 <i>k</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : k, l = 2n$
4 <i>j</i> <i>m m</i> 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
4 <i>i</i> <i>m m</i> 2	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
4 <i>h</i> <i>m 2 m</i>	$0, y, \frac{1}{2}$	$0, \bar{y}, \frac{1}{2}$			no extra conditions
4 <i>g</i> <i>m 2 m</i>	$0, y, 0$	$0, \bar{y}, 0$			no extra conditions
4 <i>f</i> <i>2 m m</i>	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$			no extra conditions
4 <i>e</i> <i>2 m m</i>	$x, 0, 0$	$\bar{x}, 0, 0$			no extra conditions
2 <i>d</i> <i>m m m</i>	$\frac{1}{2}, 0, \frac{1}{2}$				no extra conditions
2 <i>c</i> <i>m m m</i>	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
2 <i>b</i> <i>m m m</i>	$0, \frac{1}{2}, \frac{1}{2}$				no extra conditions
2 <i>a</i> <i>m m m</i>	$0, 0, 0$				no extra conditions

Symmetry of special projectionsAlong $[001] c2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along $[100] c2mm$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$ Along $[010] c2mm$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at $0, y, 0$ **Maximal non-isomorphic subgroups**

I	[2] <i>Imm</i> 2 (44)	(1; 2; 7; 8)+	IIa	[2] <i>Pmnn</i> (59)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Im2m</i> (<i>Imm</i> 2, 44)	(1; 3; 6; 8)+		[2] <i>Pmnm</i> (<i>Pmnn</i> , 59)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>I2mm</i> (<i>Imm</i> 2, 44)	(1; 4; 6; 7)+		[2] <i>Pnmm</i> (<i>Pmnn</i> , 59)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>I222</i> (23)	(1; 2; 3; 4)+		[2] <i>Pnmm</i> (58)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>I112/m</i> (<i>C2/m</i> , 12)	(1; 2; 5; 6)+		[2] <i>Pnmm</i> (<i>Pnmm</i> , 58)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>I12/m1</i> (<i>C2/m</i> , 12)	(1; 3; 5; 7)+		[2] <i>Pmnn</i> (<i>Pnmm</i> , 58)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>I2/m11</i> (<i>C2/m</i> , 12)	(1; 4; 5; 8)+		[2] <i>Pnnn</i> (48)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
				[2] <i>Pmmm</i> (47)	1; 2; 3; 4; 5; 6; 7; 8
			IIb	none	

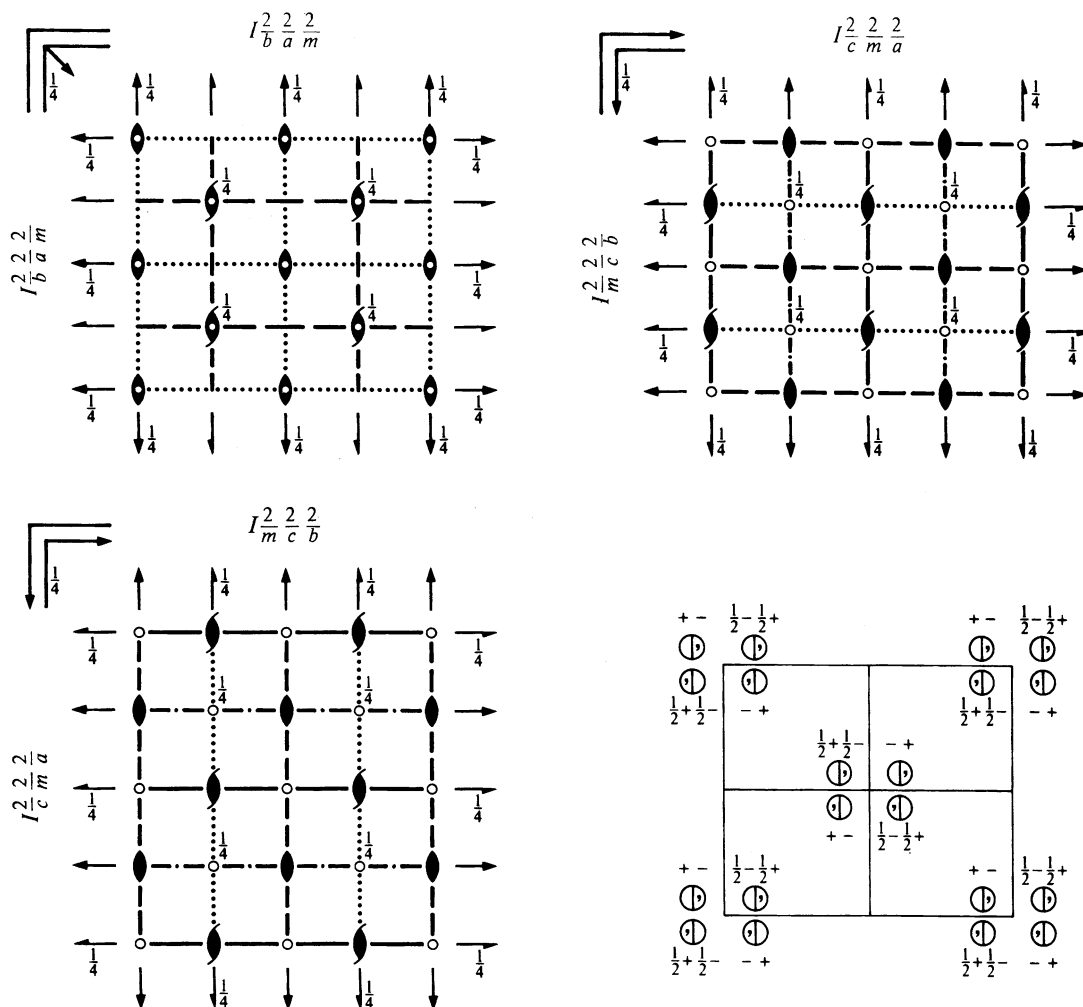
(Continued on preceding page)

$Ibam$
 D_{2h}^{26}
 mmm

Orthorhombic

No. 72

 $I 2/b 2/a 2/m$

 Patterson symmetry $Immm$

Origin at centre ($2/m$) at $cc2/m$
Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$
Symmetry operations

 For $(0,0,0)+$ set

- | | | | |
|-----------------------|-----------------|---|---|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) 2 $(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) m $x,y,0$ | (7) a $x, \frac{1}{4}, z$ | (8) b $\frac{1}{4}, y, z$ |

 For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|---|---------------------------|---------------------------|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2 $0, y, \frac{1}{4}$ | (4) 2 $x, 0, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (7) c $x, 0, z$ | (8) c $0, y, z$ |

Maximal isomorphic subgroups of lowest index
IIc [3] $Ibam$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (72); [3] $Ibam$ ($\mathbf{c}' = 3\mathbf{c}$) (72)

Minimal non-isomorphic supergroups
I [2] $I4/mcm$ (140)

II [2] $Cmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (65); [2] $Aemm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Cmme$, 67); [2] $Bmem$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Cmme$, 67)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16	<i>k</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	$hkl : h + k + l = 2n$ $Ok l : k, l = 2n$ $h0l : h, l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
8	<i>j</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	Special: as above, plus no extra conditions
8	<i>i</i> .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$	$hkl : l = 2n$
8	<i>h</i> .. 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hkl : l = 2n$
8	<i>g</i> . 2 .	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$	$0, y, \frac{3}{4}$	$hkl : l = 2n$
8	<i>f</i> 2 ..	$x, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$x, 0, \frac{3}{4}$	$hkl : l = 2n$
8	<i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : k, l = 2n$
4	<i>d</i> .. $2/m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$			$hkl : l = 2n$
4	<i>c</i> .. $2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : l = 2n$
4	<i>b</i> 2 2 2	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$			$hkl : l = 2n$
4	<i>a</i> 2 2 2	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$

Symmetry of special projections

Along $[001]$ $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along $[010]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] <i>Ib2m</i> (<i>Ima2</i> , 46)	(1; 3; 6; 8)+
	[2] <i>I2am</i> (<i>Ima2</i> , 46)	(1; 4; 6; 7)+
	[2] <i>Iba2</i> (45)	(1; 2; 7; 8)+
	[2] <i>I222</i> (23)	(1; 2; 3; 4)+
	[2] <i>I12/a1</i> (<i>C2/c</i> , 15)	(1; 3; 5; 7)+
	[2] <i>I2/b11</i> (<i>C2/c</i> , 15)	(1; 4; 5; 8)+
	[2] <i>I112/m</i> (<i>C2/m</i> , 12)	(1; 2; 5; 6)+
IIa	[2] <i>Pcan</i> (<i>Pbcn</i> , 60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pbcn</i> (60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pbcm</i> (57)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pcam</i> (<i>Pbcm</i> , 57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pccn</i> (56)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] <i>Pbam</i> (55)	1; 2; 3; 4; 5; 6; 7; 8
	[2] <i>Pban</i> (50)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
[2] <i>Pccm</i> (49)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	
IIb	none	

(Continued on preceding page)

Ibca

D_{2h}^{27}

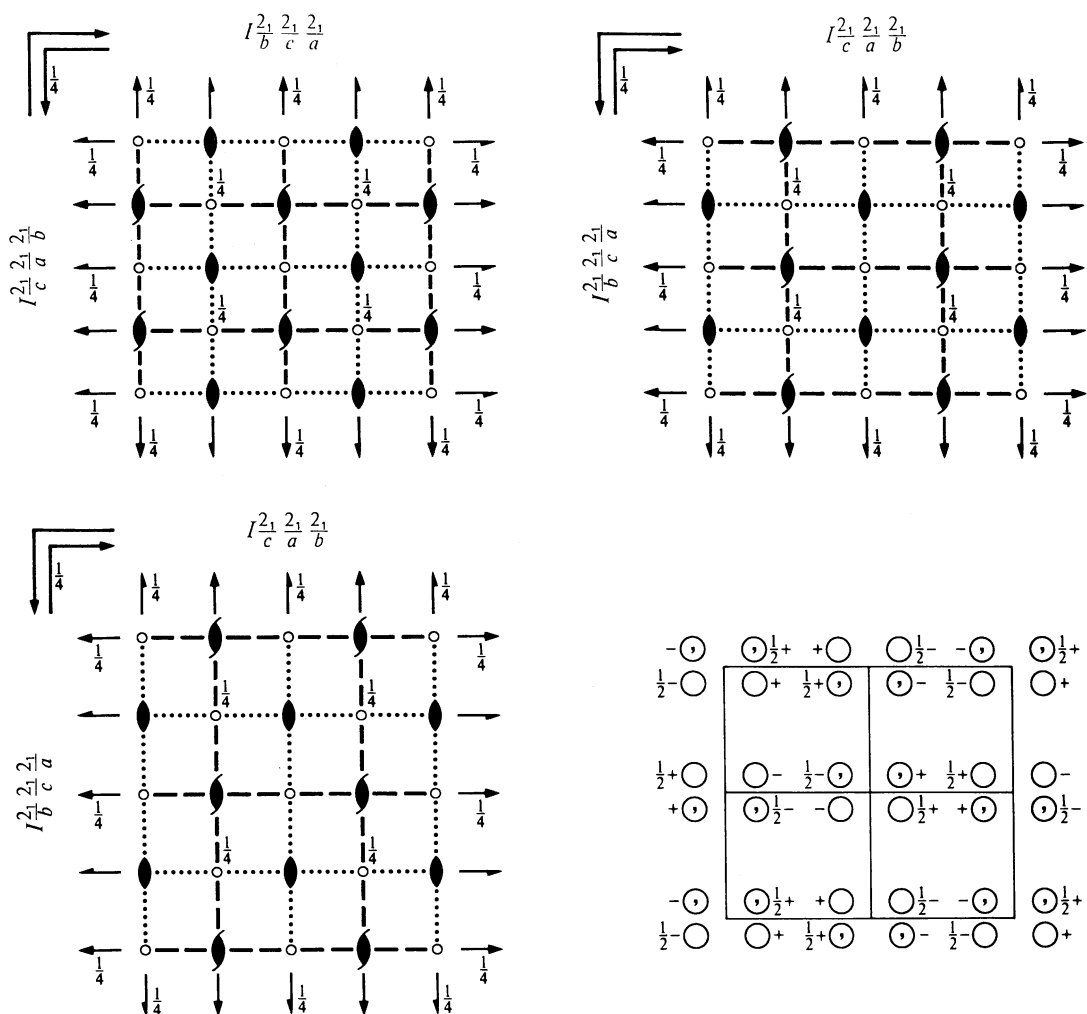
mmm

Orthorhombic

No. 73

$I 2_1/b 2_1/c 2_1/a$

Patterson symmetry *Immm*



Origin at $\bar{1}$ at *cab*

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-------------------------|--|--|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) <i>a</i> $x, y, \frac{1}{4}$ | (7) <i>c</i> $x, \frac{1}{4}, z$ | (8) <i>b</i> $\frac{1}{4}, y, z$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

- | | | | |
|---|-----------------------------|-----------------------------|-----------------------------|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, \frac{1}{4}, z$ | (3) 2 $\frac{1}{4}, y, 0$ | (4) 2 $x, 0, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) <i>b</i> $x, y, 0$ | (7) <i>a</i> $x, 0, z$ | (8) <i>c</i> $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ +				General:
16 <i>f</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$hkl : h+k+l=2n$ $Ok_l : k,l=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8 <i>e</i> ..2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},z+\frac{1}{2}$	$hkl : l=2n$
8 <i>d</i> .2.	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y,\frac{1}{2}$	$hkl : k=2n$
8 <i>c</i> 2..	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$hkl : h=2n$
8 <i>b</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$hkl : k,l=2n$
8 <i>a</i> $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$hkl : k,l=2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0,z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at x,0,0

Along [010] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0,y,0

Maximal non-isomorphic subgroups

I	[2] <i>Ibc2</i> (<i>Iba2</i> , 45)	(1; 2; 7; 8)+
	[2] <i>Ib2a</i> (<i>Iba2</i> , 45)	(1; 3; 6; 8)+
	[2] <i>I2ca</i> (<i>Iba2</i> , 45)	(1; 4; 6; 7)+
	[2] <i>I2</i> , $2_1, 2_1$ (24)	(1; 2; 3; 4)+
	[2] <i>I112/a</i> (<i>C2/c</i> , 15)	(1; 2; 5; 6)+
	[2] <i>I12/c1</i> (<i>C2/c</i> , 15)	(1; 3; 5; 7)+
	[2] <i>I2/b11</i> (<i>C2/c</i> , 15)	(1; 4; 5; 8)+
IIa	[2] <i>Pbca</i> (61)	1; 2; 3; 4; 5; 6; 7; 8
	[2] <i>Pcab</i> (<i>Pbca</i> , 61)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] <i>Pcaa</i> (<i>Pcca</i> , 54)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] <i>Pccb</i> (<i>Pcca</i> , 54)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] <i>Pbab</i> (<i>Pcca</i> , 54)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] <i>Pbcb</i> (<i>Pcca</i> , 54)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] <i>Pbaa</i> (<i>Pcca</i> , 54)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] <i>Pcca</i> (54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] *Ibca* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (73)

Minimal non-isomorphic supergroups

I [2] *I4*, */acd* (142); [3] *Ia $\bar{3}$ (206)*

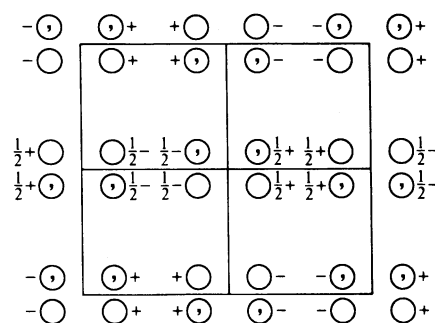
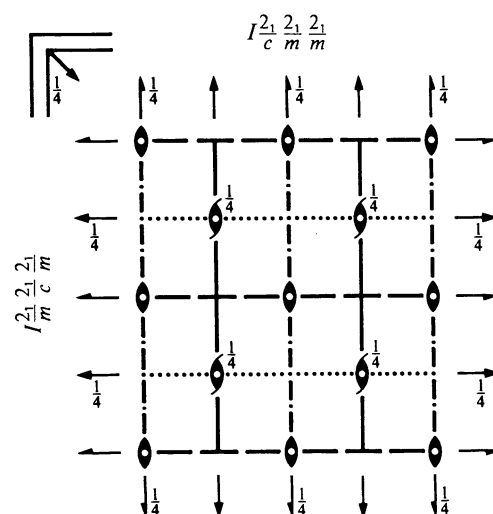
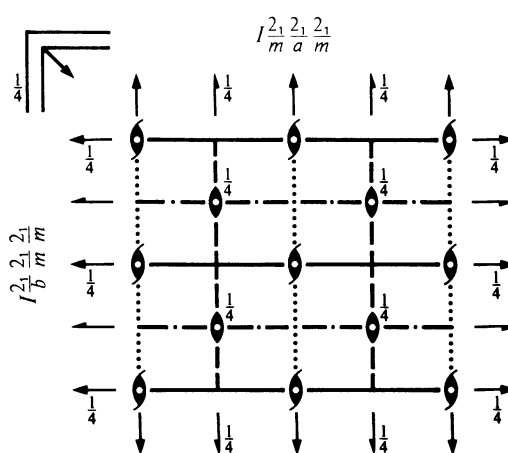
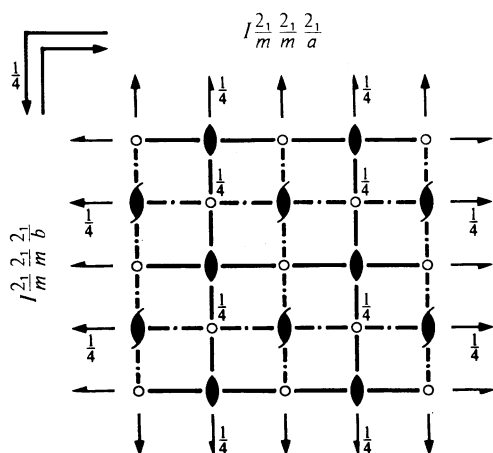
II [2] *Aemm* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Cmme*, 67); [2] *Bmem* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (*Cmme*, 67); [2] *Cmme* ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)

Imma
 D_{2h}^{28}
mmm

Orthorhombic

No. 74

 $I 2_1/m 2_1/m 2_1/a$

 Patterson symmetry *Immm*

Origin at centre ($2/m$) at $2/m2_1/nb$
Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$
Symmetry operations

 For $(0,0,0)^+$ set

- | | | | |
|-------------------------|---------------------------|---------------------------------------|-------------------|
| (1) 1 | (2) 2 $0, \frac{1}{4}, z$ | (3) 2 $(0, \frac{1}{2}, 0)$ $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) b $x, y, 0$ | (7) m $x, \frac{1}{4}, z$ | (8) m $0, y, z$ |

 For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|---|---|--|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2 $(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) a $x, y, \frac{1}{4}$ | (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |

Maximal isomorphic subgroups of lowest index
IIc $[3]Imma$ ($a' = 3a$ or $b' = 3b$) (74); $[3]Imma$ ($c' = 3c$) (74)

Minimal non-isomorphic supergroups
I $[2]I4_1/amd$ (141)

II $[2]Ammm$ ($a' = \frac{1}{2}a$) ($Cmmm$, 65); $[2]Bmmm$ ($b' = \frac{1}{2}b$) ($Cmmm$, 65); $[2]Cmme$ ($c' = \frac{1}{2}c$) (67)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	General:
16 <i>j</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$ (2) $\bar{x}, \bar{y} + \frac{1}{2}, z$ (6) $x, y + \frac{1}{2}, \bar{z}$ (3) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (7) $x, \bar{y} + \frac{1}{2}, z$ (4) x, \bar{y}, \bar{z} (8) \bar{x}, y, z	$hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h, k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
8 <i>i</i> . <i>m</i> .	$x, \frac{1}{4}, z$ $\bar{x}, \frac{1}{4}, z$ $\bar{x}, \frac{3}{4}, \bar{z}$ $x, \frac{3}{4}, \bar{z}$	Special: as above, plus no extra conditions
8 <i>h</i> <i>m</i> . .	$0, y, z$ $0, \bar{y} + \frac{1}{2}, z$ $0, y + \frac{1}{2}, \bar{z}$ $0, \bar{y}, \bar{z}$	no extra conditions
8 <i>g</i> .2 .	$\frac{1}{4}, y, \frac{1}{4}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h = 2n$
8 <i>f</i> 2 . .	$x, 0, 0$ $\bar{x}, \frac{1}{2}, 0$ $\bar{x}, 0, 0$ $x, \frac{1}{2}, 0$	$hkl : k = 2n$
4 <i>e</i> <i>m m</i> 2	$0, \frac{1}{4}, z$ $0, \frac{3}{4}, \bar{z}$	no extra conditions
4 <i>d</i> .2/ <i>m</i> .	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h = 2n$
4 <i>c</i> .2/ <i>m</i> .	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h = 2n$
4 <i>b</i> 2/ <i>m</i> . .	$0, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h = 2n$
4 <i>a</i> 2/ <i>m</i> . .	$0, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h = 2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0, 0, z

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $Im2b$ ($Ima2$, 46)	(1; 3; 6; 8)+
	[2] $I2mb$ ($Ima2$, 46)	(1; 4; 6; 7)+
	[2] $Imm2$ (44)	(1; 2; 7; 8)+
	[2] $I2_12_12_1$ (24)	(1; 2; 3; 4)+
	[2] $I112/b$ ($C2/c$, 15)	(1; 2; 5; 6)+
	[2] $I12/m1$ ($C2/m$, 12)	(1; 3; 5; 7)+
	[2] $I2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
IIa	[2] $Pnma$ (62)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmnb$ ($Pnma$, 62)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pnmb$ ($Pmna$, 53)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pnna$ (52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pnnb$ ($Pnna$, 52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmma$ (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pmmb$ ($Pmma$, 51)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

(Continued on preceding page)

$P4$

C_4^1

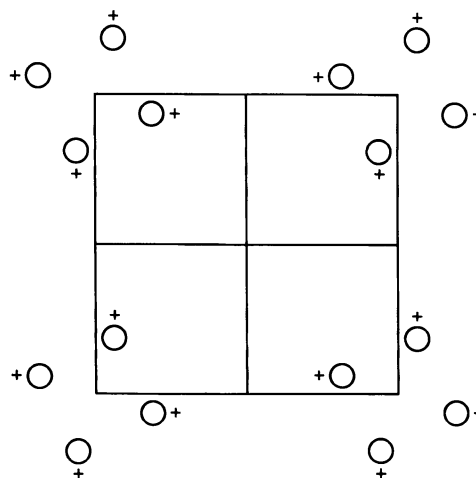
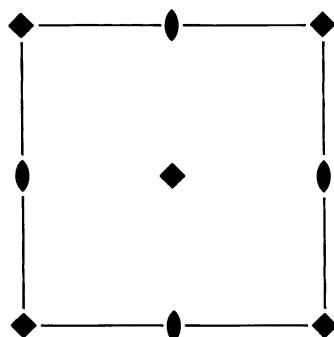
4

Tetragonal

No. 75

$P4$

Patterson symmetry $P4/m$



Origin on 4

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) 2 0,0,z (3) 4⁺ 0,0,z (4) 4⁻ 0,0,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 <i>d</i> 1	(1) x,y,z (2) \bar{x},\bar{y},z (3) \bar{y},x,z (4) y,\bar{x},z	General: no conditions Special: $hkl : h+k=2n$
2 <i>c</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$	no extra conditions
1 <i>b</i> 4..	$\frac{1}{2}, \frac{1}{2}, z$	no extra conditions
1 <i>a</i> 4..	$0, 0, z$	no extra conditions

Symmetry of special projections

Along [001] $p4$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0,0,z

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P2(3)$ 1; 2

IIa none

IIb [2] $P4_2(\mathbf{c}' = 2\mathbf{c})(77)$; [2] $F4(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c})(I4, 79)$

Maximal isomorphic subgroups of lowest index

IIc [2] $P4(\mathbf{c}' = 2\mathbf{c})(75)$; [2] $C4(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b})(P4, 75)$

Minimal non-isomorphic supergroups

I [2] $P4/m(83)$; [2] $P4/n(85)$; [2] $P422(89)$; [2] $P4_22(90)$; [2] $P4mm(99)$; [2] $P4bm(100)$; [2] $P4cc(103)$; [2] $P4nc(104)$

II [2] $I4(79)$

Tetragonal

4

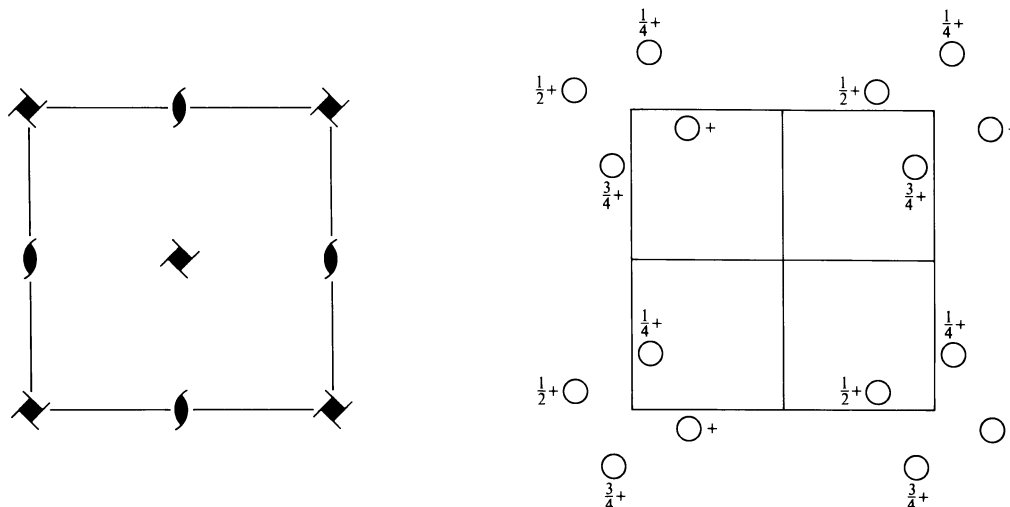
C_4^2

$P4_1$

Patterson symmetry $P4/m$

$P4_1$

No. 76



Origin on 4_1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{1}{4})$ $0,0,z$ (4) $4^-(0,0,\frac{3}{4})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 <i>a</i> 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{y},x,z+\frac{1}{4}$ (4) $y,\bar{x},z+\frac{3}{4}$	General: $00l : l = 4n$

Symmetry of special projections

Along $[001]$ $p4$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$	Along $[100]$ $p1g1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$	Along $[110]$ $p1g1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,x,0$
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Maximal non-isomorphic subgroups

I $[2]P2_1(4)$ 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2]C4_1(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b})(P4_1, 76)$; $[3]P4_3(\mathbf{c}' = 3\mathbf{c})(78)$; $[5]P4_1(\mathbf{c}' = 5\mathbf{c})(76)$

Minimal non-isomorphic supergroups

I $[2]P4_122(91)$; $[2]P4_12_12(92)$

II $[2]I4_1(80)$; $[2]P4_2(\mathbf{c}' = \frac{1}{2}\mathbf{c})(77)$

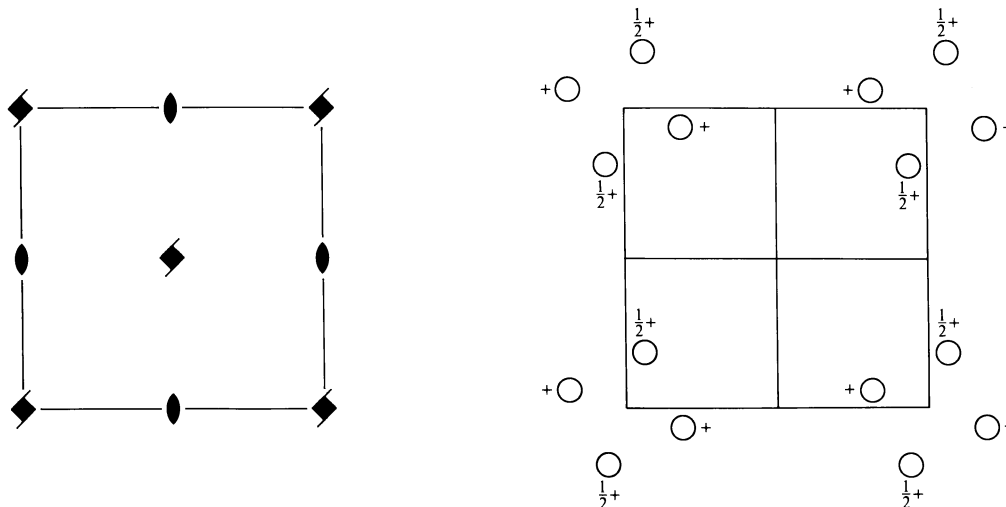
$P4_2$
 C_4^3

4

Tetragonal

No. 77

 $P4_2$

 Patterson symmetry $P4/m$

 Origin on 2 on 4_2

 Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

 (1) 1 (2) 2 $0, 0, z$ (3) $4^+(0, 0, \frac{1}{2}) 0, 0, z$ (4) $4^-(0, 0, \frac{1}{2}) 0, 0, z$

 Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (3)

Positions

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

4	<i>d</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{y}, x, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$	
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 $00l : l = 2n$

2	<i>c</i>	2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$			
---	----------	-----	---------------------	-----------------------------------	--	--	--

Special: as above, plus

 $hkl : h + k + l = 2n$

2	<i>b</i>	2..	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			
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 $hkl : l = 2n$

2	<i>a</i>	2..	$0, 0, z$	$0, 0, z + \frac{1}{2}$			
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 $hkl : l = 2n$

Symmetry of special projections

 Along $[001] p4$
 $\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

 Along $[100] p1m1$
 $\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

 Along $[110] p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I $[2] P2 (3) \quad 1; 2$
IIa none

IIb $[2] P4_3 (\mathbf{c}' = 2\mathbf{c}) (78)$; $[2] P4_1 (\mathbf{c}' = 2\mathbf{c}) (76)$; $[2] F4_1 (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I4_1, 80)$

Maximal isomorphic subgroups of lowest index

IIc $[2] C4_2 (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P4_2, 77)$; $[3] P4_2 (\mathbf{c}' = 3\mathbf{c}) (77)$

Minimal non-isomorphic supergroups

I $[2] P4_2/m (84)$; $[2] P4_2/n (86)$; $[2] P4_2 22 (93)$; $[2] P4_2 2_1 2 (94)$; $[2] P4_2 cm (101)$; $[2] P4_2 nm (102)$; $[2] P4_2 mc (105)$;
 $[2] P4_2 bc (106)$
II $[2] I4 (79)$; $[2] P4 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (75)$

Tetragonal

4

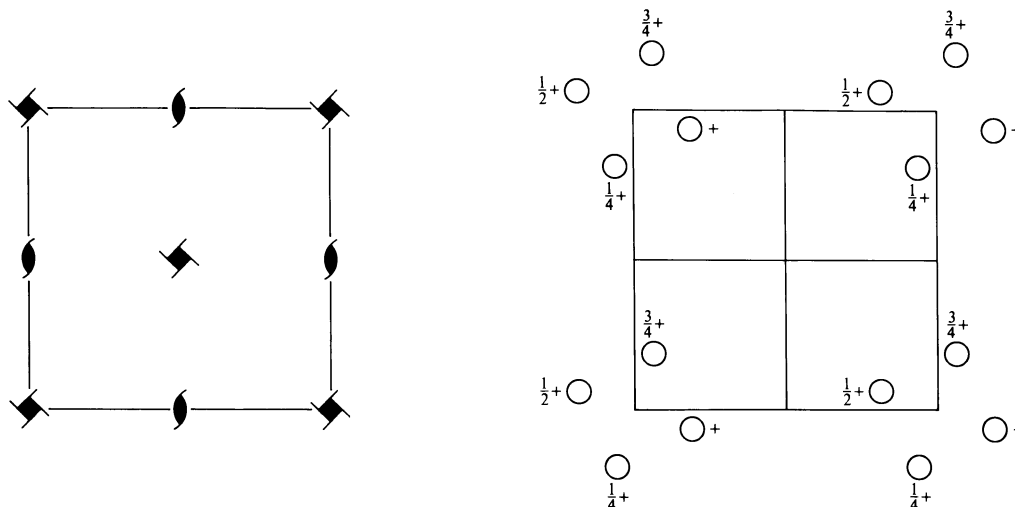
C_4^4

$P4_3$

Patterson symmetry $P4/m$

$P4_3$

No. 78



Origin on 4_3

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0, 0, \frac{1}{2})$ 0, 0, z (3) $4^+(0, 0, \frac{3}{4})$ 0, 0, z (4) $4^-(0, 0, \frac{1}{4})$ 0, 0, z

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 a 1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{3}{4}$	(4) $y, \bar{x}, z + \frac{1}{4}$	General: $00l : l = 4n$

Symmetry of special projections

Along [001] $p4$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [100] $p1g1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [110] $p1g1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$
--	--	---

Maximal non-isomorphic subgroups

I [2] $P2_1(4)$ 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_3(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b})(P4_3, 78)$; [3] $P4_1(\mathbf{c}' = 3\mathbf{c})(76)$; [5] $P4_3(\mathbf{c}' = 5\mathbf{c})(78)$

Minimal non-isomorphic supergroups

I [2] $P4_3, 22(95)$; [2] $P4_3, 2_1, 2(96)$

II [2] $I4_1(80)$; [2] $P4_2(\mathbf{c}' = \frac{1}{2}\mathbf{c})(77)$

$I4$

C_4^5

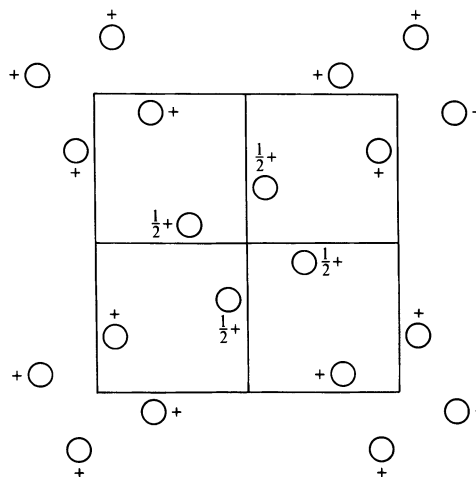
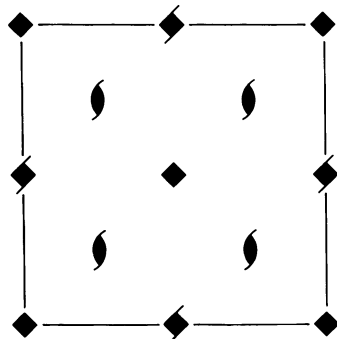
4

Tetragonal

No. 79

$I4$

Patterson symmetry $I4/m$



Origin on 4

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)^+$ set

- (1) 1 (2) $2 \ 0,0,z$ (3) $4^+ \ 0,0,z$ (4) $4^- \ 0,0,z$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) $2(0,0,\frac{1}{2}) \ \frac{1}{4}, \frac{1}{4}, z$ (3) $4^+(0,0,\frac{1}{2}) \ 0, \frac{1}{2}, z$ (4) $4^-(0,0,\frac{1}{2}) \ \frac{1}{2}, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$				General:
8 <i>c</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{y}, x, z	(4) y, \bar{x}, z	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
4 <i>b</i> 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$			Special: as above, plus $hkl : l = 2n$
2 <i>a</i> 4..	$0, 0, z$				no extra conditions

Symmetry of special projections

Along $[001] p4$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$
 Origin at $0, 0, z$

Along $[100] c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[110] p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $I2(C2, 5)$ (1; 2)+

IIa [2] $P4_2(77)$ 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4(75)$ 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4(\mathbf{c}' = 3\mathbf{c})(79)$; [5] $I4(\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})(79)$

Minimal non-isomorphic supergroups

I [2] $I4/m(87)$; [2] $I422(97)$; [2] $I4mm(107)$; [2] $I4cm(108)$

II [2] $C4(\mathbf{c}' = \frac{1}{2}\mathbf{c})(P4, 75)$

$I4_1$

C_4^6

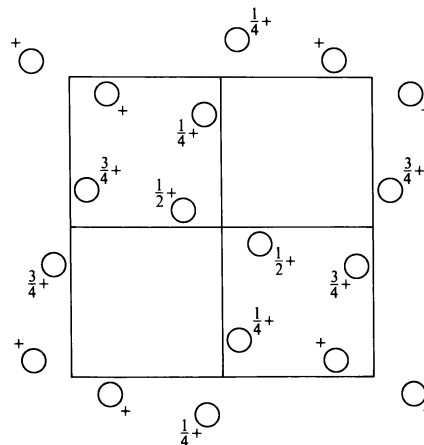
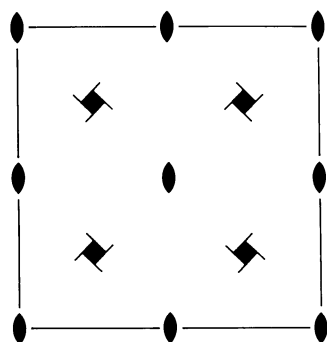
4

Tetragonal

No. 80

$I4_1$

Patterson symmetry $I4/m$



Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)^+$ set

- (1) 1 (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$ (3) $4^+(0,0,\frac{1}{4}) \quad -\frac{1}{4}, \frac{1}{4}, z$ (4) $4^-(0,0,\frac{3}{4}) \quad \frac{1}{4}, -\frac{1}{4}, z$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) $2 \quad 0,0,z$ (3) $4^+(0,0,\frac{3}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ (4) $4^-(0,0,\frac{1}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		(0,0,0)+	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$			General:
8	b 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 4n$ $h00 : h = 2n$
4	a 2..	0, 0, z	$0, \frac{1}{2}, z + \frac{1}{4}$			Special: as above, plus $hkl : l = 2n + 1$ or $2h + l = 4n$

Symmetry of special projections

Along [001] $p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $c1m1$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $I2(C2, 5)$ (1; 2)+

IIa [2] $P4_3(78)$ 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

[2] $P4_1(76)$ 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1(c' = 3c)$ (80); [5] $I4_1(a' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})$ (80)

Minimal non-isomorphic supergroups

I [2] $I4_1/a$ (88); [2] $I4_1 22$ (98); [2] $I4_1 md$ (109); [2] $I4_1 cd$ (110)

II [2] $C4_2(c' = \frac{1}{2}c)$ ($P4_2, 77$)

$P\bar{4}$

S_4^1

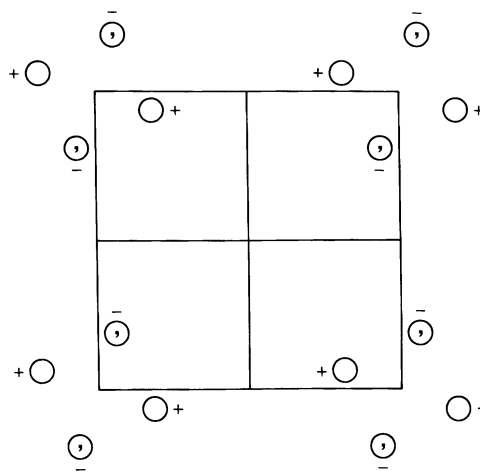
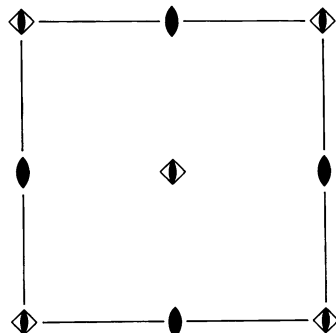
$\bar{4}$

Tetragonal

No. 81

$P\bar{4}$

Patterson symmetry $P4/m$



Origin at $\bar{4}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- (1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z; 0,0,0$ (4) $\bar{4}^-$ $0,0,z; 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 <i>h</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) y, \bar{x}, \bar{z} (4) \bar{y}, x, \bar{z}	General: no conditions Special:
2 <i>g</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$	$hk0 : h + k = 2n$
2 <i>f</i> 2..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
2 <i>e</i> 2..	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
1 <i>d</i> $\bar{4}$..	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	no extra conditions
1 <i>c</i> $\bar{4}$..	$\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions
1 <i>b</i> $\bar{4}$..	$0, 0, \frac{1}{2}$	no extra conditions
1 <i>a</i> $\bar{4}$..	$0, 0, 0$	no extra conditions

Symmetry of special projections

Along $[001]$ $p4$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[110]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P2(3)$ 1; 2

IIa none

IIb [2] $F\bar{4}(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I\bar{4}, 82)$

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}(\mathbf{c}' = 2\mathbf{c}) (81)$; [2] $C\bar{4}(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P\bar{4}, 81)$

Minimal non-isomorphic supergroups

I [2] $P4/m(83)$; [2] $P4_2/m(84)$; [2] $P4/n(85)$; [2] $P4_2/n(86)$; [2] $P\bar{4}2m(111)$; [2] $P\bar{4}2c(112)$; [2] $P\bar{4}2_1m(113)$; [2] $P\bar{4}2_1c(114)$; [2] $P\bar{4}m2(115)$; [2] $P\bar{4}c2(116)$; [2] $P\bar{4}b2(117)$; [2] $P\bar{4}n2(118)$

II [2] $I\bar{4}(82)$

$I\bar{4}$

S_4^2

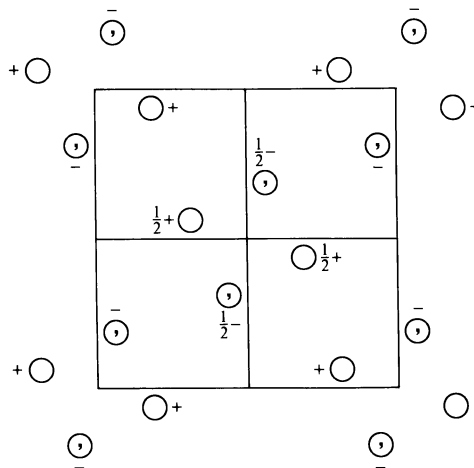
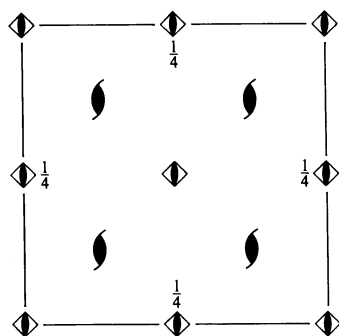
$\bar{4}$

Tetragonal

No. 82

$I\bar{4}$

Patterson symmetry $I4/m$



Origin at $\bar{4}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0,0,0)^+$ set

- (1) 1 (2) $2\ 0,0,z$ (3) $\bar{4}^+ 0,0,z; 0,0,0$ (4) $\bar{4}^- 0,0,z; 0,0,0$

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) $2(0,0,\frac{1}{2})\ \frac{1}{4}, \frac{1}{4}, z$ (3) $\bar{4}^+ \frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ (4) $\bar{4}^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
8 <i>g</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) y,\bar{x},\bar{z}	(4) \bar{y},x,\bar{z}	$hkl : h+k+l = 2n$ $hk0 : h+k = 2n$ $0kl : k+l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
4 <i>f</i> 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			Special: no extra conditions
4 <i>e</i> 2..	$0, 0, z$	$0, 0, \bar{z}$			
2 <i>d</i> $\bar{4}$..	$0, \frac{1}{2}, \frac{3}{4}$				
2 <i>c</i> $\bar{4}$..	$0, \frac{1}{2}, \frac{1}{4}$				
2 <i>b</i> $\bar{4}$..	$0, 0, \frac{1}{2}$				
2 <i>a</i> $\bar{4}$..	$0, 0, 0$				

Symmetry of special projections

Along $[001] p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[100] c1m1$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along $[110] p1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I $[2]I2(C2, 5) (1; 2)+$

IIa $[2]P\bar{4}(81) 1; 2; 3; 4$

$[2]P\bar{4}(81) 1; 2; (3; 4) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[3]I\bar{4}(c' = 3c)(82); [5]I\bar{4}(a' = a + 2b, b' = -2a + b \text{ or } a' = a - 2b, b' = 2a + b)(82)$

Minimal non-isomorphic supergroups

I $[2]I4/m(87); [2]I4_1/a(88); [2]I\bar{4}m2(119); [2]I\bar{4}c2(120); [2]I\bar{4}2m(121); [2]I\bar{4}2d(122)$

II $[2]C\bar{4}(c' = \frac{1}{2}c)(P\bar{4}, 81)$

$P4/m$

C_{4h}^1

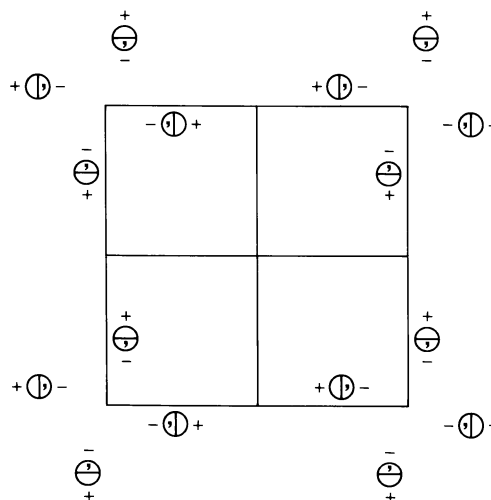
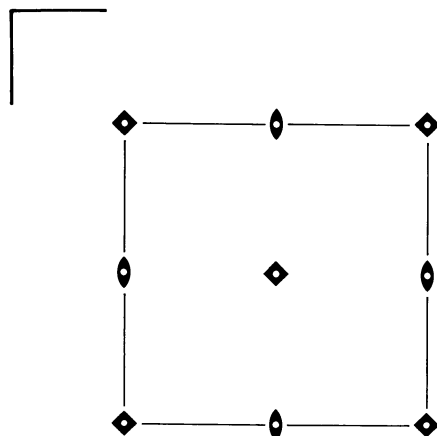
$4/m$

Tetragonal

No. 83

$P4/m$

Patterson symmetry $P4/m$



Origin at centre ($4/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------|-----------------|--------------------------------|--------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) $\bar{1}$ $0,0,0$ | (6) m $x,y,0$ | (7) $\bar{4}^+$ $0,0,z; 0,0,0$ | (8) $\bar{4}^-$ $0,0,z; 0,0,0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>l</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$ (2) \bar{x}, \bar{y}, z (6) x, y, \bar{z} (3) \bar{y}, x, z (7) y, \bar{x}, \bar{z} (4) y, \bar{x}, z (8) \bar{y}, x, \bar{z}	General: no conditions Special:
4 <i>k</i> $m..$	$x, y, \frac{1}{2}$ $\bar{x}, \bar{y}, \frac{1}{2}$ $\bar{y}, x, \frac{1}{2}$ $y, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>j</i> $m..$	$x, y, 0$ $\bar{x}, \bar{y}, 0$ $\bar{y}, x, 0$ $y, \bar{x}, 0$	no extra conditions
4 <i>i</i> $2..$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, \bar{z}$	$hkl : h + k = 2n$
2 <i>h</i> $4..$	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
2 <i>g</i> $4..$	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
2 <i>f</i> $2/m..$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>e</i> $2/m..$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : h + k = 2n$
1 <i>d</i> $4/m..$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	no extra conditions
1 <i>c</i> $4/m..$	$\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions
1 <i>b</i> $4/m..$	$0, 0, \frac{1}{2}$	no extra conditions
1 <i>a</i> $4/m..$	$0, 0, 0$	no extra conditions

Symmetry of special projections

Along $[001] p4$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100] p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[110] p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I $[2] P\bar{4} (81)$ 1; 2; 7; 8
 $[2] P4 (75)$ 1; 2; 3; 4
 $[2] P2/m (10)$ 1; 2; 5; 6

IIa none

IIb $[2] P4_2/m (\mathbf{c}' = 2\mathbf{c}) (84)$; $[2] C4/e (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P4/n, 85)$; $[2] F4/m (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I4/m, 87)$

Maximal isomorphic subgroups of lowest index

IIc $[2] P4/m (\mathbf{c}' = 2\mathbf{c}) (83)$; $[2] C4/m (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P4/m, 83)$

Minimal non-isomorphic supergroups

I $[2] P4/mmm (123)$; $[2] P4/mcc (124)$; $[2] P4/mbm (127)$; $[2] P4/mnc (128)$
II $[2] I4/m (87)$

$P4_2/m$

C_{4h}^2

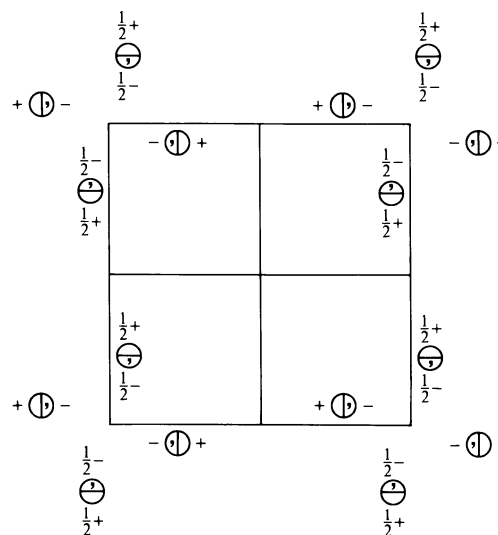
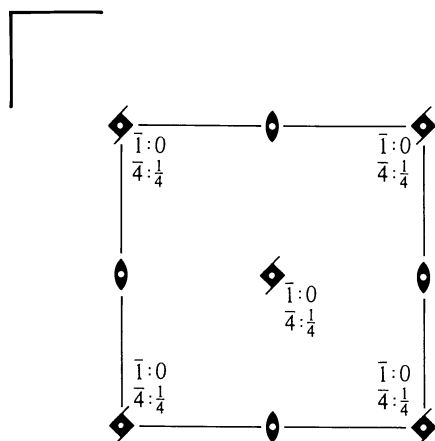
$4/m$

Tetragonal

No. 84

$P4_2/m$

Patterson symmetry $P4/m$



Origin at centre ($2/m$) on 4_2

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------|-------------------|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, 0, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $0, 0, z$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) m $x, y, 0$ | (7) $\bar{4}^+$ $0, 0, z; 0, 0, \frac{1}{4}$ | (8) $\bar{4}^-$ $0, 0, z; 0, 0, \frac{3}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
8	k 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $y, \bar{x}, \bar{z} + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, x, \bar{z} + \frac{1}{2}$	General: $00l : l = 2n$
4	j $m..$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$	Special: as above, plus no extra conditions
4	i $2..$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	h $2..$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4	g $2..$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
2	f $\bar{4}..$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2	e $\bar{4}..$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$
2	d $2/m..$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl : h + k + l = 2n$
2	c $2/m..$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	b $2/m..$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	a $2/m..$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along $[001]$ $p4$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[110]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
 [2] $P4_2$ (77) 1; 2; 3; 4
 [2] $P2/m$ (10) 1; 2; 5; 6

IIa none

IIb [2] $C4_2/e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/n$, 86)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_2/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/m$, 84); [3] $P4_2/m$ ($\mathbf{c}' = 3\mathbf{c}$) (84)

Minimal non-isomorphic supergroups

I [2] $P4_2/mmc$ (131); [2] $P4_2/mcm$ (132); [2] $P4_2/mbc$ (135); [2] $P4_2/mnm$ (136)

II [2] $I4/m$ (87); [2] $P4/m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (83)

$P4/n$

C_{4h}^3

$4/m$

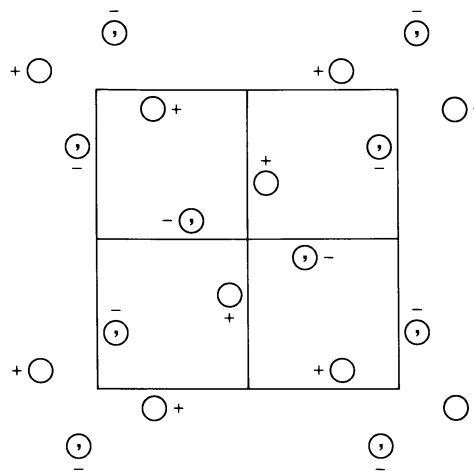
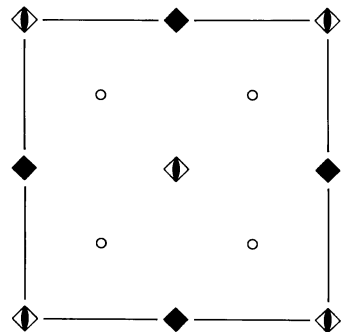
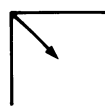
Tetragonal

No. 85

$P4/n$

Patterson symmetry $P4/m$

ORIGIN CHOICE 1



Origin at $\bar{4}$ on n , at $-\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---|--|----------------------------------|----------------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+ 0, \frac{1}{2}, z$ | (4) $4^- \frac{1}{2}, 0, z$ |
| (5) $\bar{1} \frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (7) $\bar{4}^+ 0, 0, z; 0, 0, 0$ | (8) $\bar{4}^- 0, 0, z; 0, 0, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (7) y, \bar{x}, \bar{z}	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (8) \bar{y}, x, \bar{z}	$hk0 : h + k = 2n$ $h00 : h = 2n$
					Special: as above, plus
4 <i>f</i> 2..	0, 0, z	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	0, 0, \bar{z}	$hkl : h + k = 2n$
4 <i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h, k = 2n$
2 <i>c</i> 4..	0, $\frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
2 <i>b</i> $\bar{4}$..	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> $\bar{4}$..	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}$ (81)	1; 2; 7; 8
	[2] $P4$ (75)	1; 2; 3; 4
	[2] $P2/n$ ($P2/c$, 13)	1; 2; 5; 6

IIa none

IIb [2] $P4_2/n$ ($c' = 2c$) (86)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/n$ ($c' = 2c$) (85); [5] $P4/n$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) (85)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)

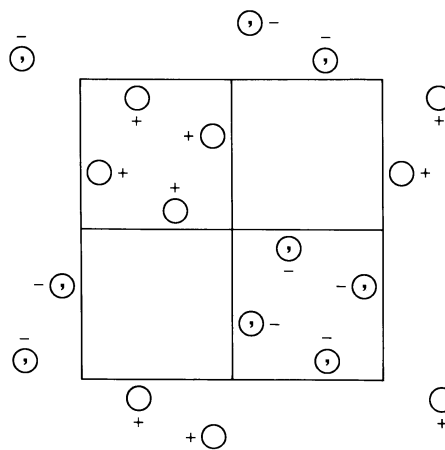
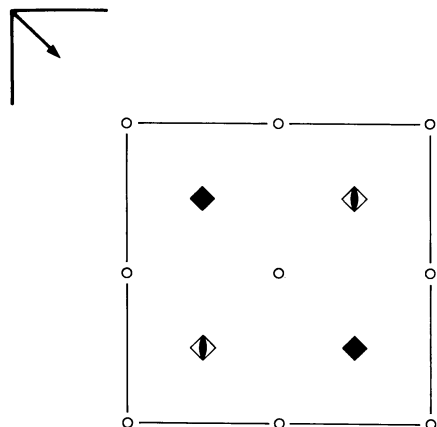
$P4/n$ C_{4h}^3 $4/m$

Tetragonal

No. 85

 $P4/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 2

Origin at $\bar{1}$ on n , at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------|--|--|--|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+ \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^- \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (7) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ | (8) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
8	<i>g</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{y} + \frac{1}{2}, x, z$ (7) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(4) $y, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, x + \frac{1}{2}, \bar{z}$	General: $hkl : h + k = 2n$ $h00 : h = 2n$ Special: as above, plus $hkl : h + k = 2n$ $hkl : h, k = 2n$ $hkl : h, k = 2n$ no extra conditions $hkl : h + k = 2n$ $hkl : h + k = 2n$
4	<i>f</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	
4	<i>e</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	
4	<i>d</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	
2	<i>c</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$			
2	<i>b</i> $\bar{4}$..	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$			
2	<i>a</i> $\bar{4}$..	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$			

Symmetry of special projections

Along [001] $p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}$ (81)	1; 2; 7; 8
	[2] $P4$ (75)	1; 2; 3; 4
	[2] $P2/n$ ($P2/c$, 13)	1; 2; 5; 6

IIa none

IIb [2] $P4_2/n$ ($\mathbf{c}' = 2\mathbf{c}$) (86)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/n$ ($\mathbf{c}' = 2\mathbf{c}$) (85); [5] $P4/n$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) (85)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)

$P4_2/n$

C_{4h}^4

$4/m$

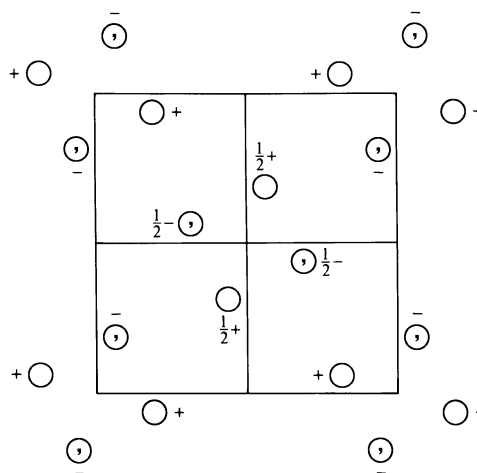
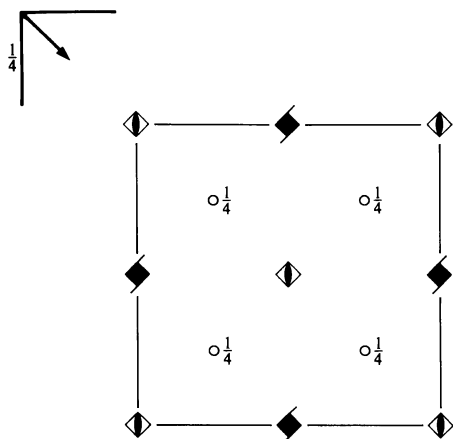
Tetragonal

No. 86

$P4_2/n$

Patterson symmetry $P4/m$

ORIGIN CHOICE 1



Origin at $\bar{4}$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---|--|--|--|
| (1) 1 | (2) $2 \ 0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2}) \ 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \ \frac{1}{2}, 0, z$ |
| (5) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, \frac{1}{4}$ | (7) $\bar{4}^+ \ 0, 0, z; \ 0, 0, 0$ | (8) $\bar{4}^- \ 0, 0, z; \ 0, 0, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) y, \bar{x}, \bar{z}	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) \bar{y}, x, \bar{z}	$hk0 : h + k = 2n$ $00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus
4 <i>f</i> 2..	0, 0, z	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	0, 0, \bar{z}	$hkl : h + k + l = 2n$
4 <i>e</i> 2..	0, $\frac{1}{2}, z$	0, $\frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$
4 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>c</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
2 <i>b</i> $\bar{4}$..	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}$..	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

- I** [2] $P\bar{4}$ (81) 1; 2; 7; 8
 [2] $P4_2$ (77) 1; 2; 3; 4
 [2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $F4_1/d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/a$, 88)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n$ ($\mathbf{c}' = 3\mathbf{c}$) (86); [5] $P4_2/n$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) (86)

Minimal non-isomorphic supergroups

I [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II [2] $C4_2/m$ ($P4_2/m$, 84); [2] $I4/m$ (87); [2] $P4/n$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (85)

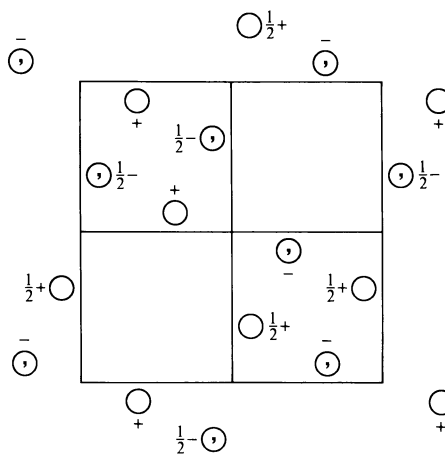
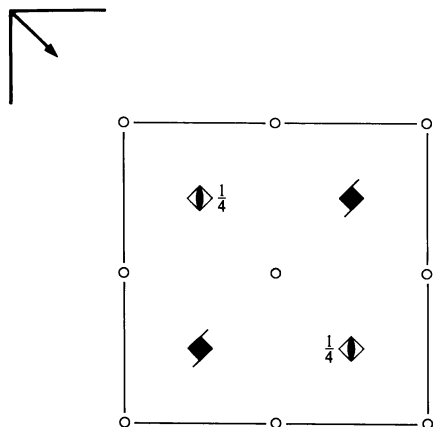
$P4_2/n$ C_{4h}^4 $4/m$

Tetragonal

No. 86

 $P4_2/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 2

Origin at $\bar{1}$ on n , at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{4}$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------|--|--|--|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) -\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, -\frac{1}{4}, z$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (7) $\bar{4}^+ \frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (8) $\bar{4}^- \frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>g</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{2}$ (4) $y + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ (5) $\bar{x}, \bar{y}, \bar{z}$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $y, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	General: $hk0 : h + k = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus $hkl : h + k + l = 2n$
4 <i>f</i> 2..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>e</i> 2..	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4 <i>d</i> $\bar{1}$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>c</i> $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
2 <i>b</i> $\bar{4}..$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}..$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along $[100]$ $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** [2] $P\bar{4}$ (81) 1; 2; 7; 8
 [2] $P4_2$ (77) 1; 2; 3; 4
 [2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $F4_1/d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/a$, 88)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n$ ($\mathbf{c}' = 3\mathbf{c}$) (86); [5] $P4_2/n$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) (86)

Minimal non-isomorphic supergroups

I [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II [2] $C4_2/m$ ($P4_2/m$, 84); [2] $I4/m$ (87); [2] $P4/n$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (85)

$I4/m$

C_{4h}^5

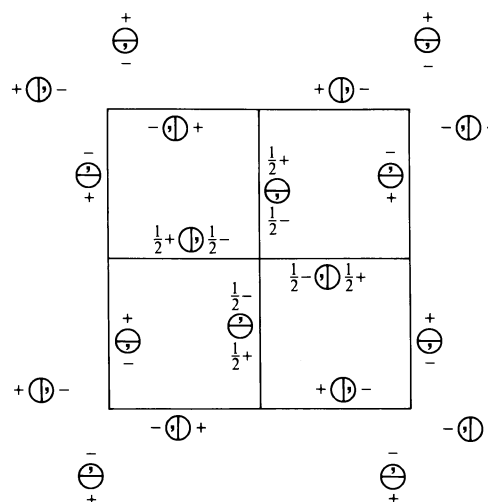
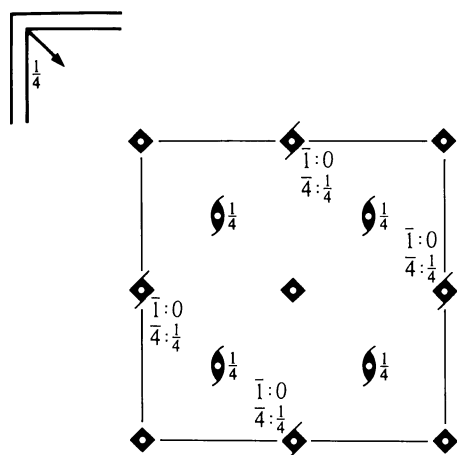
$4/m$

Tetragonal

No. 87

$I4/m$

Patterson symmetry $I4/m$



Origin at centre ($4/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)^+$ set

- | | | | |
|---------------------|-----------------------|------------------------------|------------------------------|
| (1) 1 | (2) $2 \bar{1} 0,0,z$ | (3) $4^+ 0,0,z$ | (4) $4^- 0,0,z$ |
| (5) $\bar{1} 0,0,0$ | (6) $m x,y,0$ | (7) $\bar{4}^+ 0,0,z; 0,0,0$ | (8) $\bar{4}^- 0,0,z; 0,0,0$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0,\frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{1}{2}) 0, \frac{1}{2}, z$ | (4) $4^-(0,0,\frac{1}{2}) \frac{1}{2}, 0, z$ |
| (5) $\bar{1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, \frac{1}{4}$ | (7) $\bar{4}^+ \frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (8) $\bar{4}^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$	General:
16 <i>i</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$
	(2) \bar{x}, \bar{y}, z (6) x, y, \bar{z}	Special: as above, plus
	(3) \bar{y}, x, z (7) y, \bar{x}, \bar{z}	no extra conditions
	(4) y, \bar{x}, z (8) \bar{y}, x, \bar{z}	$hkl : l=2n$
8 <i>h</i> $m..$	$x, y, 0$ $\bar{x}, \bar{y}, 0$ $\bar{y}, x, 0$ $y, \bar{x}, 0$	no extra conditions
8 <i>g</i> $2..$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, \bar{z}$	$hkl : l=2n$
8 <i>f</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : k, l=2n$
4 <i>e</i> $4..$	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
4 <i>d</i> $\bar{4}..$	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$	$hkl : l=2n$
4 <i>c</i> $2/m..$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : l=2n$
2 <i>b</i> $4/m..$	$0, 0, \frac{1}{2}$	no extra conditions
2 <i>a</i> $4/m..$	$0, 0, 0$	no extra conditions

Symmetry of special projections

Along [001] $p4$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+
	[2] $I4$ (79)	(1; 2; 3; 4)+
	[2] $I2/m$ ($C2/m$, 12)	(1; 2; 5; 6)+
IIa	[2] $P4_2/n$ (86)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4/n$ (85)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2/m$ (84)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4/m$ (83)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4/m$ ($\mathbf{c}' = 3\mathbf{c}$) (87); [5] $I4/m$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) (87)

Minimal non-isomorphic supergroups

I	[2] $I4/mmm$ (139); [2] $I4/mcm$ (140)
II	[2] $C4/m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4/m$, 83)

$I4_1/a$

C_{4h}^6

$4/m$

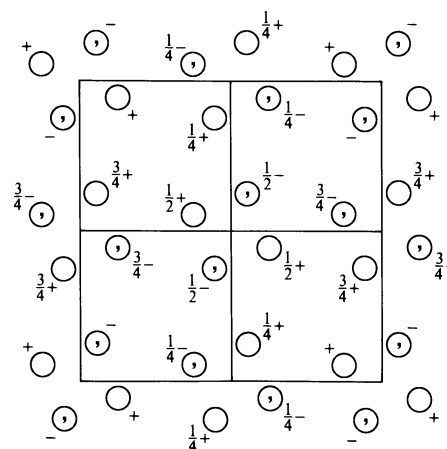
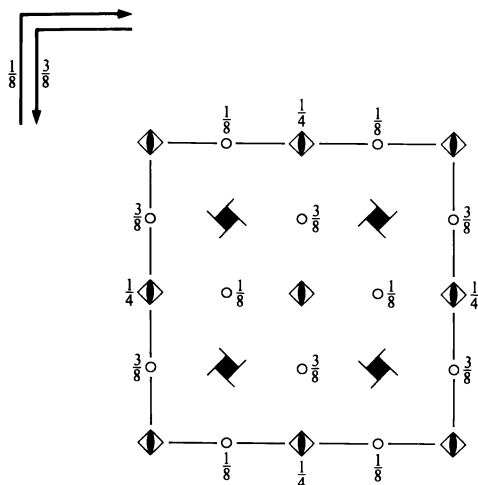
Tetragonal

No. 88

$I4_1/a$

Patterson symmetry $I4/m$

ORIGIN CHOICE 1



Origin at $\bar{4}$, at $0, -\frac{1}{4}, -\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

For $(0, 0, 0)^+$ set

- | | | | |
|---|--|---|--|
| (1) $\bar{1}$ | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{4}) \quad -\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{3}{4}) \quad \frac{1}{4}, -\frac{1}{4}, z$ |
| (5) $\bar{1} \quad 0, \frac{1}{4}, \frac{1}{8}$ | (6) $a \quad x, y, \frac{3}{8}$ | (7) $\bar{4}^+ \quad 0, 0, z; \quad 0, 0, 0$ | (8) $\bar{4}^- \quad 0, \frac{1}{2}, z; \quad 0, \frac{1}{2}, \frac{1}{4}$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|---|---------------------------------|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, 0, z$ | (3) $4^+(0, 0, \frac{3}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $\bar{1} \quad \frac{1}{4}, 0, \frac{3}{8}$ | (6) $b \quad x, y, \frac{1}{8}$ | (7) $\bar{4}^+ \quad \frac{1}{2}, 0, z; \quad \frac{1}{2}, 0, \frac{1}{4}$ | (8) $\bar{4}^- \quad 0, 0, z; \quad 0, 0, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions	
		$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$					
16	f	1	(1) x, y, z (5) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (7) y, \bar{x}, \bar{z}	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (8) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	General: $hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
8	e	2..	$0, 0, z$	$0, \frac{1}{2}, z + \frac{1}{4}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{4}$	$0, 0, \bar{z}$	Special: as above, plus $hkl : l = 2n + 1$ or $2h + l = 4n$
8	d	$\bar{1}$	$0, \frac{1}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$	$\frac{3}{4}, \frac{1}{2}, \frac{7}{8}$	$\frac{3}{4}, 0, \frac{3}{8}$	$hkl : l = 2n + 1$ or $h, k = 2n, h + k + l = 4n$
8	c	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$	$\frac{3}{4}, \frac{1}{2}, \frac{3}{8}$	$\frac{3}{4}, 0, \frac{7}{8}$	
4	b	$\bar{4}..$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{3}{4}$	$\left. \begin{array}{l} \\ \end{array} \right\}$	$hkl : l = 2n + 1$ or $2h + l = 4n$	
4	a	$\bar{4}..$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{4}$			

Symmetry of special projections

Along $[001]$ $p4$

$$\mathbf{a}' = \frac{1}{2}\mathbf{a} \quad \mathbf{b}' = \frac{1}{2}\mathbf{b}$$

Origin at $0, 0, z$

Along $[100]$ $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, \frac{3}{8}$

Along $[110]$ $p2mg$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x + \frac{1}{4}, \frac{1}{8}$

Maximal non-isomorphic subgroups

- I** $[2]I\bar{4}(82)$ (1; 2; 7; 8)+
 $[2]I4_1(80)$ (1; 2; 3; 4)+
 $[2]I2/a(C2/c, 15)$ (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

- IIc** $[3]I4_1/a(\mathbf{c}' = 3\mathbf{c})(88)$; $[5]I4_1/a(\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})(88)$

Minimal non-isomorphic supergroups

- I** $[2]I4_1/amd(141)$; $[2]I4_1/acd(142)$

- II** $[2]C4_2/a(\mathbf{c}' = \frac{1}{2}\mathbf{c})(P4_2/n, 86)$

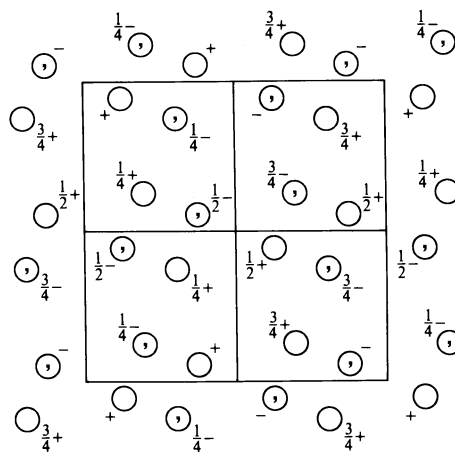
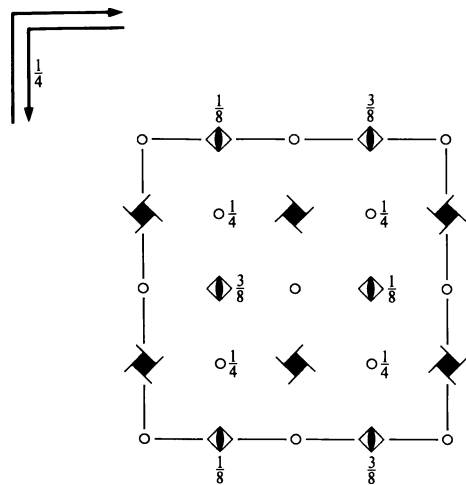
$I4_1/a$ C_{4h}^6 $4/m$

Tetragonal

No. 88

 $I4_1/a$ Patterson symmetry $I4/m$

ORIGIN CHOICE 2

**Origin** at $\bar{1}$ on glide plane b , at $0, \frac{1}{4}, \frac{1}{8}$ from $\bar{4}$ **Asymmetric unit** $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ **Symmetry operations**For $(0,0,0)^+$ set

- | | | | |
|---------------------------|--|--|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $4^+(0,0,\frac{1}{4}) \quad \frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0,0,\frac{3}{4}) \quad \frac{3}{4}, 0, z$ |
| (5) $\bar{1} \quad 0,0,0$ | (6) $a \quad x,y,\frac{1}{4}$ | (7) $\bar{4}^+ \quad \frac{1}{2}, \frac{1}{4}, z; \frac{1}{2}, \frac{1}{4}, \frac{3}{8}$ | (8) $\bar{4}^- \quad 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{1}{8}$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|---|---------------------------------|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{3}{4}) \quad -\frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0,0,\frac{1}{4}) \quad \frac{1}{4}, 0, z$ |
| (5) $\bar{1} \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $b \quad x,y,0$ | (7) $\bar{4}^+ \quad \frac{1}{2}, -\frac{1}{4}, z; \frac{1}{2}, -\frac{1}{4}, \frac{1}{8}$ | (8) $\bar{4}^- \quad 0, \frac{3}{4}, z; 0, \frac{3}{4}, \frac{3}{8}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16 <i>f</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{y} + \frac{3}{4}, x + \frac{1}{4}, z + \frac{1}{4}$ (7) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(4) $y + \frac{3}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$ (8) $\bar{y} + \frac{1}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
8 <i>e</i> 2..	$0, \frac{1}{4}, z$	$\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}$	$0, \frac{3}{4}, \bar{z}$	$\frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{3}{4}$	Special: as above, plus $hkl : l = 2n + 1$ or $2h + l = 4n$
8 <i>d</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : l = 2n + 1$ or $h, k = 2n, h + k + l = 4n$
8 <i>c</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	
4 <i>b</i> $\bar{4}..$	$0, \frac{1}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{7}{8}$			$hkl : l = 2n + 1$ or $2h + l = 4n$
4 <i>a</i> $\bar{4}..$	$0, \frac{1}{4}, \frac{1}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{8}$			

Symmetry of special projections

Along $[001]$ $p4$

$$\mathbf{a}' = \frac{1}{2}\mathbf{a} \quad \mathbf{b}' = \frac{1}{2}\mathbf{b}$$

Origin at $\frac{1}{4}, 0, z$

Along $[100]$ $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along $[110]$ $p2mg$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** $[2]I\bar{4}(82)$ (1; 2; 7; 8)+
 $[2]I4_1(80)$ (1; 2; 3; 4)+
 $[2]I2/a(C2/c, 15)$ (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

- IIc** $[3]I4_1/a(\mathbf{c}' = 3\mathbf{c})(88)$; $[5]I4_1/a(\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})(88)$

Minimal non-isomorphic supergroups

- I** $[2]I4_1/amd(141)$; $[2]I4_1/acd(142)$

- II** $[2]C4_2/a(\mathbf{c}' = \frac{1}{2}\mathbf{c})(P4_2/n, 86)$

$P422$

D_4^1

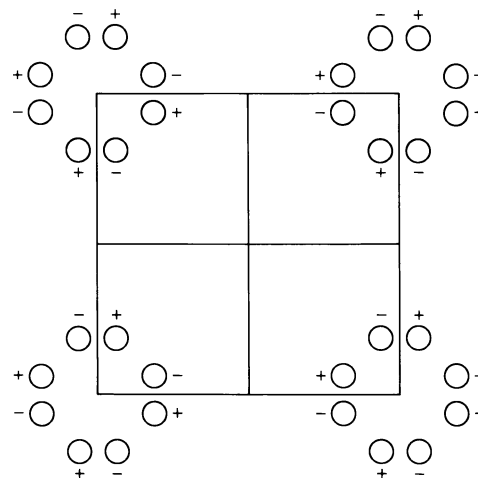
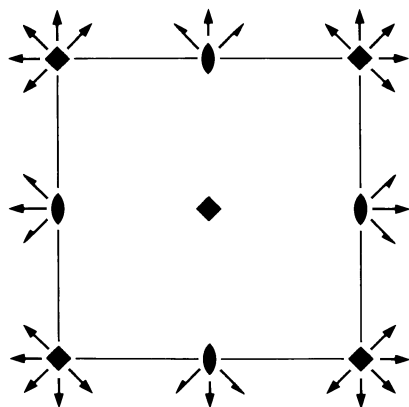
422

Tetragonal

No. 89

$P422$

Patterson symmetry $P4/mmm$



Origin at 422

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---------------|---------------|-------------------|---------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,0$ | (8) 2 $x,\bar{x},0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>p</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z}	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z}	(3) \bar{y}, x, z (7) y, x, \bar{z}	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$	no conditions
					Special:
4 <i>o</i> .2.	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4 <i>n</i> .2.	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>m</i> .2.	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>l</i> .2.	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4 <i>k</i> ..2	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>j</i> ..2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
4 <i>i</i> 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : h + k = 2n$
2 <i>h</i> 4..	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions
2 <i>g</i> 4..	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
2 <i>f</i> 222.	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>e</i> 222.	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$			$hkl : h + k = 2n$
1 <i>d</i> 422	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				no extra conditions
1 <i>c</i> 422	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
1 <i>b</i> 422	$0, 0, \frac{1}{2}$				no extra conditions
1 <i>a</i> 422	$0, 0, 0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4, 75$) 1; 2; 3; 4
 [2] $P212$ ($C222, 21$) 1; 2; 7; 8
 [2] $P221$ ($P222, 16$) 1; 2; 5; 6

IIa none

IIb [2] $P4_222$ ($\mathbf{c}' = 2\mathbf{c}$) (93); [2] $C422_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P42_12, 90$); [2] $F422$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I422, 97$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P422$ ($\mathbf{c}' = 2\mathbf{c}$) (89); [2] $C422$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P422, 89$)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/mcc$ (124); [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [3] $P432$ (207)

II [2] $I422$ (97)

$P4_2 2_1 2$

D_4^2

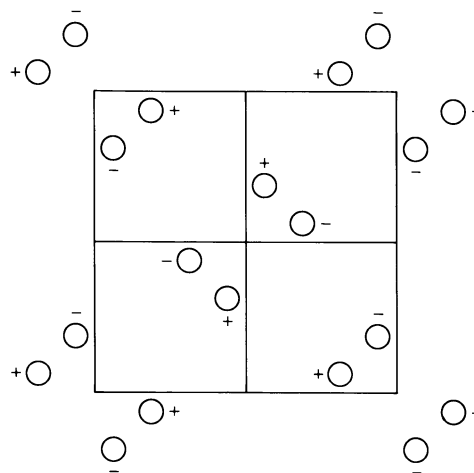
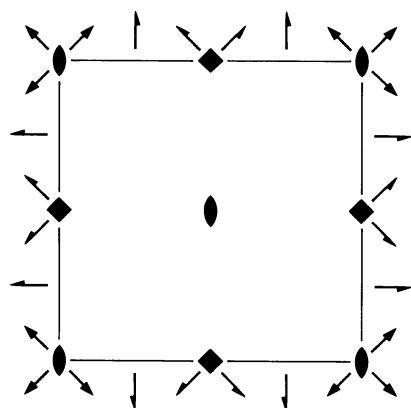
422

Tetragonal

No. 90

$P4_2 2_1 2$

Patterson symmetry $P4/mmm$



Origin at 222 at 212

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|--|--|-------------------------------|-------------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, \frac{1}{2}, z$ | (4) 4^- $\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>g</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	$hk0 : h = 2n$
	(5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(7) y, x, \bar{z}	(8) $\bar{y}, \bar{x}, \bar{z}$	
4 <i>f</i> ..2	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	Special: as above, plus $0kl : k = 2n$
4 <i>e</i> ..2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0kl : k = 2n$
4 <i>d</i> 2..	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$hkl : h + k = 2n$
2 <i>c</i> 4..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			$hk0 : h + k = 2n$
2 <i>b</i> 2.22	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> 2.22	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, \frac{1}{2}, z$

Along [100] $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4, 75$) 1; 2; 3; 4
 [2] $P212$ ($C222, 21$) 1; 2; 7; 8
 [2] $P22_11$ ($P2_12_12, 18$) 1; 2; 5; 6

IIa none

IIIb [2] $P4_22_12$ ($\mathbf{c}' = 2\mathbf{c}$) (94)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4_22_12$ ($\mathbf{c}' = 2\mathbf{c}$) (90); [9] $P4_22_12$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (90)

Minimal non-isomorphic supergroups

I [2] $P4/mbm$ (127); [2] $P4/mnc$ (128); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)
II [2] $C422$ ($P422, 89$); [2] $I422$ (97)

$P4_122$

D_4^3

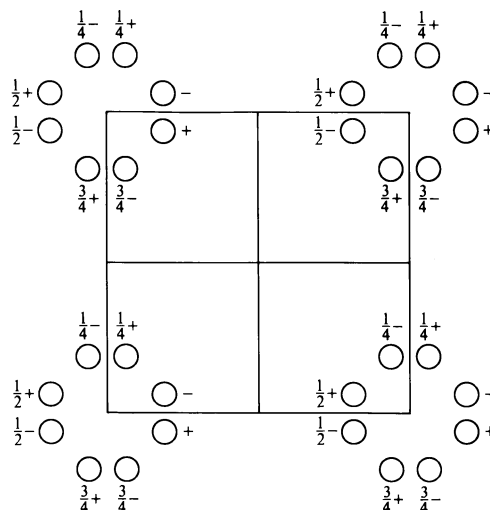
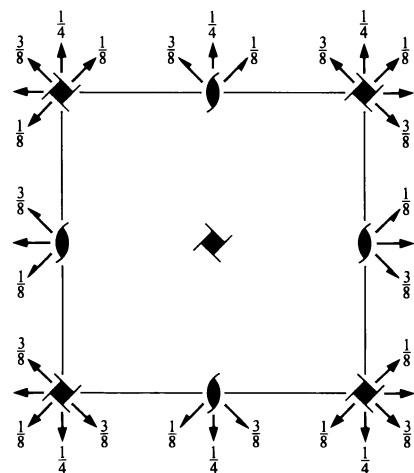
422

Tetragonal

No. 91

$P4_122$

Patterson symmetry $P4/mmm$



Origin on $2[010]$ at $4_1(1,2)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

- | | | | |
|-----------------|----------------------------------|------------------------------------|------------------------------------|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,0,z$ | (3) $4^+(0,0,\frac{1}{4})$ $0,0,z$ | (4) $4^-(0,0,\frac{3}{4})$ $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,\frac{1}{4}$ | (7) 2 $x,x,\frac{1}{8}$ | (8) 2 $x,\bar{x},\frac{1}{8}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>d</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z}	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{1}{4}$ (7) $y, x, \bar{z} + \frac{3}{4}$	(4) $y, \bar{x}, z + \frac{3}{4}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{4}$	General: $00l : l = 4n$ Special: as above, plus
4 <i>c</i> . . 2	$x, x, \frac{3}{8}$	$\bar{x}, \bar{x}, \frac{7}{8}$	$\bar{x}, x, \frac{5}{8}$	$x, \bar{x}, \frac{1}{8}$	$0kl : l = 2n + 1$ or $l = 4n$
4 <i>b</i> . 2 .	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	$\bar{y}, \frac{1}{2}, \frac{1}{4}$	$y, \frac{1}{2}, \frac{3}{4}$	$hhl : l = 2n + 1$ or $l = 4n$
4 <i>a</i> . 2 .	$0, y, 0$	$0, \bar{y}, \frac{1}{2}$	$\bar{y}, 0, \frac{1}{4}$	$y, 0, \frac{3}{4}$	$hhl : l = 2n + 1$ or $l = 4n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, \frac{1}{4}$

Along [110] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, \frac{3}{8}$

Maximal non-isomorphic subgroups

I [2] $P4_111$ ($P4_1$, 76) 1; 2; 3; 4
[2] $P2_121$ ($P222_1$, 17) 1; 2; 5; 6
[2] $P2_112$ ($C222_1$, 20) 1; 2; 7; 8

IIa none

IIb [2] $C4_122_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_12_12$, 92)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_122$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_122$, 91); [3] $P4_322$ ($\mathbf{c}' = 3\mathbf{c}$) (95); [5] $P4_122$ ($\mathbf{c}' = 5\mathbf{c}$) (91)

Minimal non-isomorphic supergroups

I none

II [2] $I4_122$ (98); [2] $P4_122$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (93)

$P4_12_12$

D_4^4

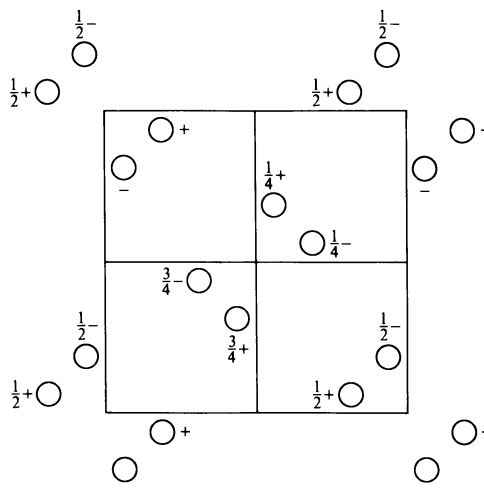
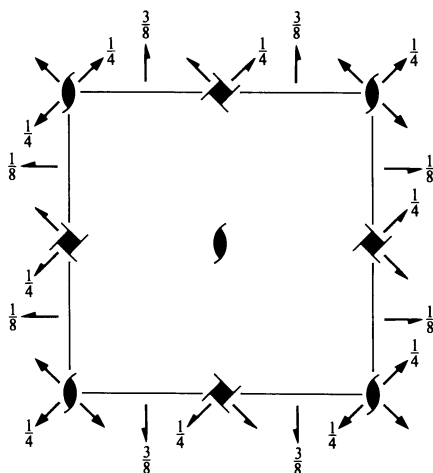
422

Tetragonal

No. 92

$P4_12_12$

Patterson symmetry $P4/mmm$



Origin on $2[110]$ at $2_11(1,2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

- | | | | |
|--|--|--|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{4})$ $0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{3}{4})$ $\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{8}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{3}{8}$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>b</i> 1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{4}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$	$00l : l = 4n$ $h00 : h = 2n$
	(5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{3}{4}$	(7) y, x, \bar{z}	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	Special: as above, plus
4 <i>a</i> .. 2	$x, x, 0$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$0kl : l = 2n + 1$ or $2k + l = 4n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, \frac{1}{2}, z$

Along [100] $p2gg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, \frac{3}{8}$

Along [110] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_111$ ($P4_1, 76$) 1; 2; 3; 4
 [2] $P2_112$ ($C222_1, 20$) 1; 2; 7; 8
 [2] $P2_12_11$ ($P2_12_12_1, 19$) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_32_12$ ($\mathbf{c}' = 3\mathbf{c}$) (96); [5] $P4_12_12$ ($\mathbf{c}' = 5\mathbf{c}$) (92); [9] $P4_12_12$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (92)

Minimal non-isomorphic supergroups

I [3] $P4_132$ (213)

II [2] $C4_122$ ($P4_122, 91$); [2] $I4_122$ (98); [2] $P4_22_12$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (94)

$P4_222$

D_4^5

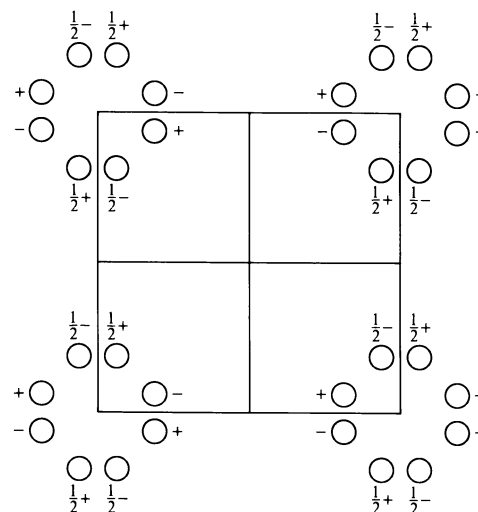
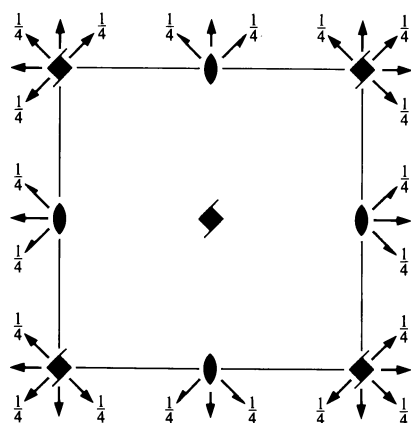
422

Tetragonal

No. 93

$P4_222$

Patterson symmetry $P4/mmm$



Origin at 222 at 4_221

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---------------|---------------|------------------------------------|------------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ | (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>p</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z}	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z}	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	General: $00l : l = 2n$
4 <i>o</i> . . 2	$x, x, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, x, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$	Special: as above, plus $0kl : l = 2n$
4 <i>n</i> . . 2	$x, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, x, \frac{3}{4}$	$x, \bar{x}, \frac{3}{4}$	$0kl : l = 2n$
4 <i>m</i> . 2 .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$hhl : l = 2n$
4 <i>l</i> . 2 .	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, 0$	$0, \bar{x}, 0$	$hhl : l = 2n$
4 <i>k</i> . 2 .	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$hhl : l = 2n$
4 <i>j</i> . 2 .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$hhl : l = 2n$
4 <i>i</i> 2 . .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>h</i> 2 . .	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4 <i>g</i> 2 . .	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
2 <i>f</i> 2 . 22	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2 <i>e</i> 2 . 22	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$
2 <i>d</i> 2 2 2 .	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl : h + k + l = 2n$
2 <i>c</i> 2 2 2 .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2 <i>b</i> 2 2 2 .	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2 <i>a</i> 2 2 2 .	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P4_2 11 (P4_2, 77)$ 1; 2; 3; 4
 [2] $P2 12 (C222, 21)$ 1; 2; 7; 8
 [2] $P2 21 (P222, 16)$ 1; 2; 5; 6

IIa none

IIb [2] $P4_3 22 (\mathbf{c}' = 2\mathbf{c}) (95)$; [2] $P4_1 22 (\mathbf{c}' = 2\mathbf{c}) (91)$; [2] $C4_2 22_1 (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P4_2 2_1 2, 94)$;
 [2] $F4_1 22 (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I4_1 22, 98)$

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_2 22 (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (P4_2 22, 93)$; [3] $P4_2 22 (\mathbf{c}' = 3\mathbf{c}) (93)$

Minimal non-isomorphic supergroups

I [2] $P4_2/mmc (131)$; [2] $P4_2/mcm (132)$; [2] $P4_2/nbc (133)$; [2] $P4_2/nnm (134)$; [3] $P4_2 32 (208)$

II [2] $I4 22 (97)$; [2] $P4 22 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (89)$

$P4_2 2_1 2$

D_4^6

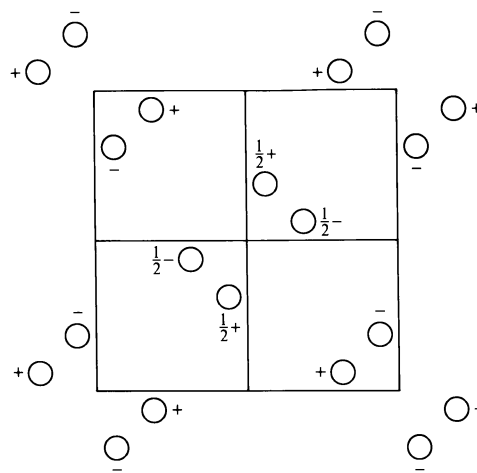
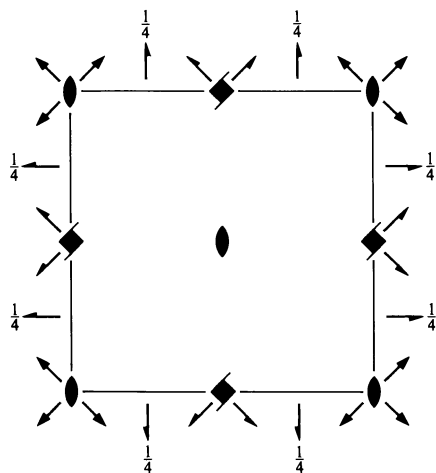
422

Tetragonal

No. 94

$P4_2 2_1 2$

Patterson symmetry $P4/mmm$



Origin at 222 at 212

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|--|--|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) y, x, \bar{z}	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$	General: $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus $0kl : k + l = 2n$ $hkl : l = 2n$ $hk0 : h + k = 2n$ $hkl : h + k + l = 2n$ $hkl : h + k + l = 2n$ $hkl : h + k + l = 2n$
4 <i>f</i> ..2	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0kl : k + l = 2n$
4 <i>e</i> ..2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0kl : k + l = 2n$
4 <i>d</i> 2..	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$ $hk0 : h + k = 2n$
4 <i>c</i> 2..	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$hkl : h + k + l = 2n$
2 <i>b</i> 2.22	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2 <i>a</i> 2.22	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, \frac{1}{2}, z$

Along [100] $p2mg$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [110] $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** [2] $P4_211$ ($P4_2, 77$) 1; 2; 3; 4
 [2] $P212$ ($C222, 21$) 1; 2; 7; 8
 [2] $P22_11$ ($P2_12_12, 18$) 1; 2; 5; 6

IIa none

IIb [2] $P4_32_12$ ($\mathbf{c}' = 2\mathbf{c}$) (96); [2] $P4_12_12$ ($\mathbf{c}' = 2\mathbf{c}$) (92)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_22_12$ ($\mathbf{c}' = 3\mathbf{c}$) (94); [9] $P4_22_12$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (94)

Minimal non-isomorphic supergroups

I [2] $P4_2/mbc$ (135); [2] $P4_2/mnm$ (136); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II [2] $C4_222$ ($P4_222, 93$); [2] $I422$ (97); [2] $P4_22_12$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (90)

$P4_322$

D_4^7

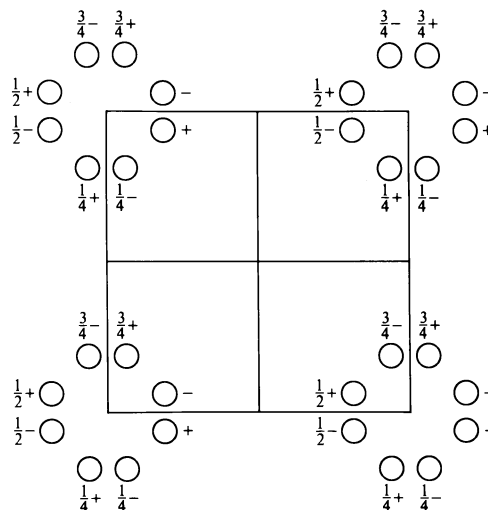
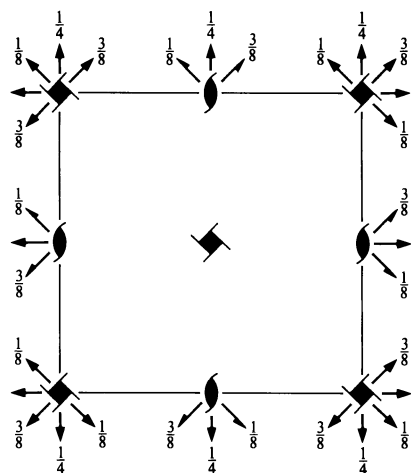
422

Tetragonal

No. 95

$P4_322$

Patterson symmetry $P4/mmm$



Origin on $2[010]$ at $4_3(1,2)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

- | | | | |
|-----------------|----------------------------------|------------------------------------|------------------------------------|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,0,z$ | (3) $4^+(0,0,\frac{3}{4})$ $0,0,z$ | (4) $4^-(0,0,\frac{1}{4})$ $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,\frac{1}{4}$ | (7) 2 $x,x,\frac{1}{8}$ | (8) 2 $x,\bar{x},\frac{3}{8}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>d</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z}	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{3}{4}$ (7) $y, x, \bar{z} + \frac{1}{4}$	(4) $y, \bar{x}, z + \frac{1}{4}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{3}{4}$	General: $00l : l = 4n$ Special: as above, plus
4 <i>c</i> . . 2	$x, x, \frac{5}{8}$	$\bar{x}, \bar{x}, \frac{1}{8}$	$\bar{x}, x, \frac{3}{8}$	$x, \bar{x}, \frac{7}{8}$	$0kl : l = 2n + 1$ or $l = 4n$
4 <i>b</i> . 2 .	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	$\bar{y}, \frac{1}{2}, \frac{3}{4}$	$y, \frac{1}{2}, \frac{1}{4}$	$hhl : l = 2n + 1$ or $l = 4n$
4 <i>a</i> . 2 .	$0, y, 0$	$0, \bar{y}, \frac{1}{2}$	$\bar{y}, 0, \frac{3}{4}$	$y, 0, \frac{1}{4}$	$hhl : l = 2n + 1$ or $l = 4n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, \frac{1}{4}$

Along [110] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, \frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $P4_311$ ($P4_3, 78$) 1; 2; 3; 4
[2] $P2_112$ ($C222_1, 20$) 1; 2; 7; 8
[2] $P2_121$ ($P222_1, 17$) 1; 2; 5; 6

IIa none

IIb [2] $C4_322_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_32_12, 96$)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_322$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_322, 95$); [3] $P4_122$ ($\mathbf{c}' = 3\mathbf{c}$) (91); [5] $P4_322$ ($\mathbf{c}' = 5\mathbf{c}$) (95)

Minimal non-isomorphic supergroups

I none

II [2] $I4_122$ (98); [2] $P4_322$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (93)

$P4_3 2_1 2$

D_4^8

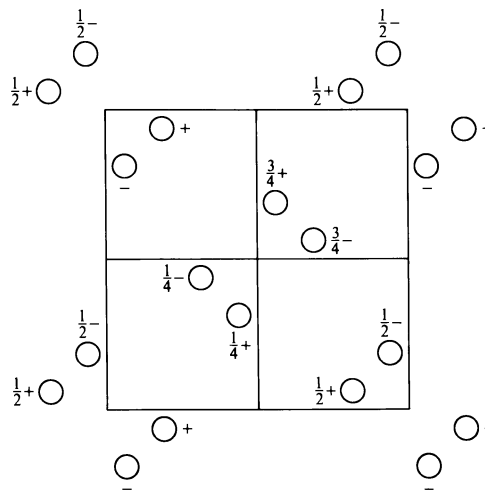
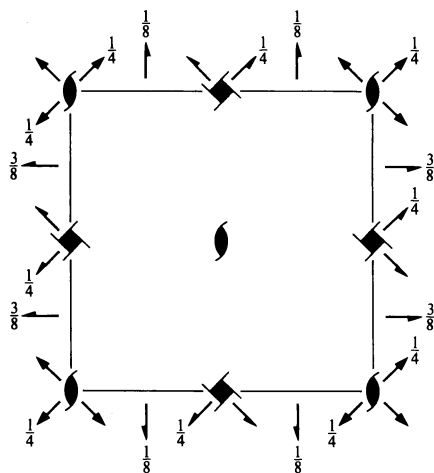
422

Tetragonal

No. 96

$P4_3 2_1 2$

Patterson symmetry $P4/mmm$



Origin on $2[110]$ at $2_1 1(1,2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

- | | | | |
|--|--|--|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,0,z$ | (3) $4^+(0,0,\frac{3}{4})$ $0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{2},0,z$ |
| (5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{3}{8}$ | (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{8}$ | (7) 2 $x,x,0$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>b</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{3}{4}$	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{3}{4}$ (7) y, x, \bar{z}	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{4}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	$00l : l = 4n$ $h00 : h = 2n$
4 <i>a</i> .. 2	$x, x, 0$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	Special: as above, plus $0kl : l = 2n + 1$ or $2k + l = 4n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

Along [100] $p2gg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{4}, \frac{1}{8}$

Along [110] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_3 11$ ($P4_3, 78$) 1; 2; 3; 4
[2] $P2_1 12$ ($C222_1, 20$) 1; 2; 7; 8
[2] $P2_1 2_1 1$ ($P2_1 2_1 2_1, 19$) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_1 2_1 2$ ($\mathbf{c}' = 3\mathbf{c}$) (92); [5] $P4_3 2_1 2$ ($\mathbf{c}' = 5\mathbf{c}$) (96); [9] $P4_3 2_1 2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (96)

Minimal non-isomorphic supergroups

I [3] $P4_3 32$ (212)

II [2] $C4_3 22$ ($P4_3 22, 95$); [2] $I4_1 22$ (98); [2] $P4_2 2_1 2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (94)

*I*422

D_4^9

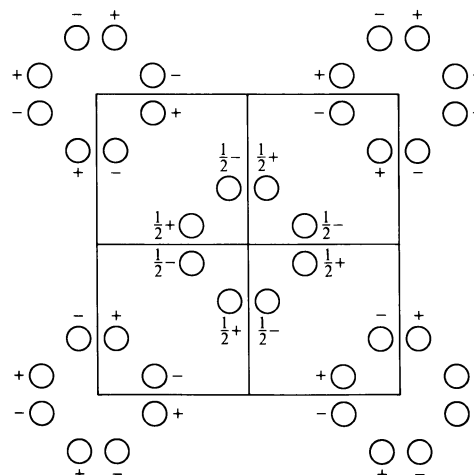
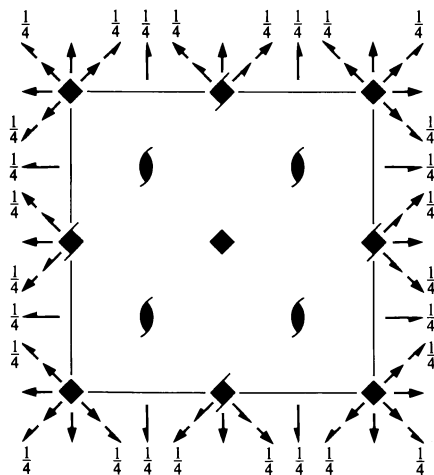
422

Tetragonal

No. 97

*I*422

Patterson symmetry *I*4/*m**m*



Origin at 422

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-------------|-------------|--------------------------|--------------------------|
| (1) 1 | (2) 2 0,0,z | (3) 4 ⁺ 0,0,z | (4) 4 ⁻ 0,0,z |
| (5) 2 0,y,0 | (6) 2 x,0,0 | (7) 2 x,x,0 | (8) 2 x,x̄,0 |

For (1/2, 1/2, 1/2)+ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0) \frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) x, \frac{1}{4}, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, \frac{1}{4}$ | (8) $2 x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	General:
16 <i>k</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (3) \bar{y}, x, z (7) y, x, \bar{z} (4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8 <i>j</i> ..2	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$Ok l : k = 2n$
8 <i>i</i> .2.	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$	no extra conditions
8 <i>h</i> .2.	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$	no extra conditions
8 <i>g</i> ..2	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, x, 0$ $x, \bar{x}, 0$	no extra conditions
8 <i>f</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$
4 <i>e</i> 4..	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
4 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$	$hkl : l = 2n$
4 <i>c</i> 222.	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : l = 2n$
2 <i>b</i> 422	$0, 0, \frac{1}{2}$	no extra conditions
2 <i>a</i> 422	$0, 0, 0$	no extra conditions

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I411$ ($I4, 79$)	(1; 2; 3; 4)+
	[2] $I221$ ($I222, 23$)	(1; 2; 5; 6)+
	[2] $I212$ ($F222, 22$)	(1; 2; 7; 8)+
IIa	[2] $P4_2, 2$ (94)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2, 2$ (93)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2, 2$ (90)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
IIIb	none	

Maximal isomorphic subgroups of lowest index

IIIc [3] $I422$ ($\mathbf{c}' = 3\mathbf{c}$) (97); [9] $I422$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (97)

Minimal non-isomorphic supergroups

I [2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $F432$ (209); [3] $I432$ (211)

II [2] $C422$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P422, 89$)

$I4_122$

D_4^{10}

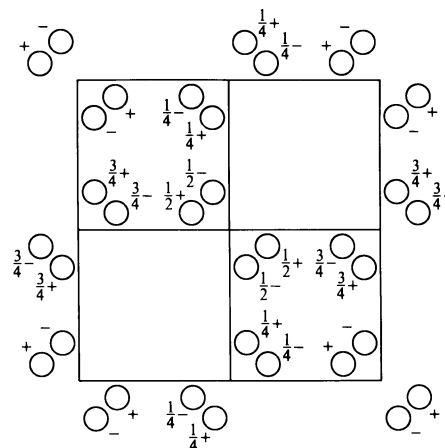
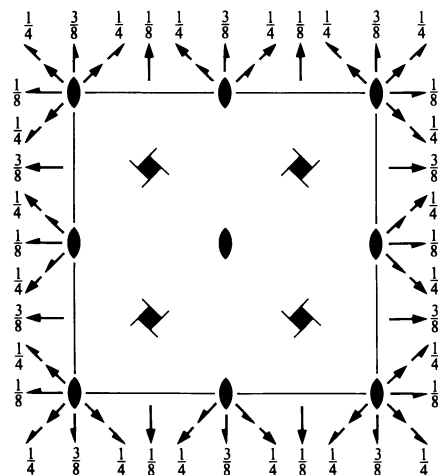
422

Tetragonal

No. 98

$I4_122$

Patterson symmetry $I4/mmm$



Origin at 222 at 212

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---|--|---|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{1}{4}) \quad -\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{3}{4}) \quad \frac{1}{4}, -\frac{1}{4}, z$ |
| (5) $2 \quad \frac{1}{4}, y, \frac{3}{8}$ | (6) $2 \quad x, \frac{1}{4}, \frac{1}{8}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, \frac{1}{4}$ | (8) $2 \quad x, \bar{x}, 0$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, 0, z$ | (3) $4^+(0,0,\frac{3}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{1}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{8}$ | (6) $2(\frac{1}{2}, 0, 0) \quad x, 0, \frac{3}{8}$ | (7) $2 \quad x, x, 0$ | (8) $2 \quad x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	(0,0,0) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ +	General:
16 <i>g</i> 1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) \bar{y},\bar{x},\bar{z}	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=4n$ $h00 : h=2n$
8 <i>f</i> .2.	$x,\frac{1}{4},\frac{1}{8}$ $\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$ $\frac{3}{4},\bar{x},\frac{7}{8}$	$hhl : l=4n$
8 <i>e</i> ..2	$\bar{x},x,0$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},x,\frac{3}{4}$	$0kl : k=2n+1$ or $l=4n$
8 <i>d</i> ..2	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},\bar{x},\frac{3}{4}$	$0kl : k=2n+1$ or $l=4n$
8 <i>c</i> 2..	$0,0,z$ $0,\frac{1}{2},z+\frac{1}{4}$ $\frac{1}{2},0,\bar{z}+\frac{3}{4}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl : l=2n+1$ or $2h+l=4n$
4 <i>b</i> 2.22	$0,0,\frac{1}{2}$ $0,\frac{1}{2},\frac{3}{4}$	$hkl : l=2n+1$ or $2h+l=4n$
4 <i>a</i> 2.22	$0,0,0$ $0,\frac{1}{2},\frac{1}{4}$	$hkl : l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x,0,\frac{3}{8}$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I4_1 11 (I4_1, 80)$	(1; 2; 3; 4) +
	[2] $I2_1 21 (I2_1, 24)$	(1; 2; 5; 6) +
	[2] $I2_1 12 (F222, 22)$	(1; 2; 7; 8) +
IIa	[2] $P4_3 2, 2 (96)$	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_3 2, 2 (95)$	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_1 2, 2 (92)$	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_1 2, 2 (91)$	1; 2; 3; 4; 5; 6; 7; 8

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1 22 (\mathbf{c}' = 3\mathbf{c}) (98)$; [9] $I4_1 22 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (98)$

Minimal non-isomorphic supergroups

I [2] $I4_1/amd (141)$; [2] $I4_1/acd (142)$; [3] $F4_1 32 (210)$; [3] $I4_1 32 (214)$

II [2] $C4_2 22 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P4_2 22, 93)$

$P4mm$

C_{4v}^1

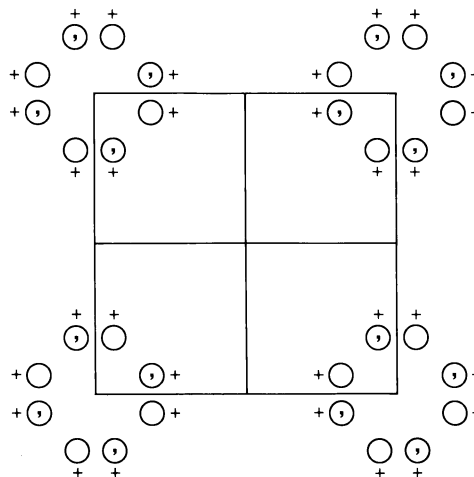
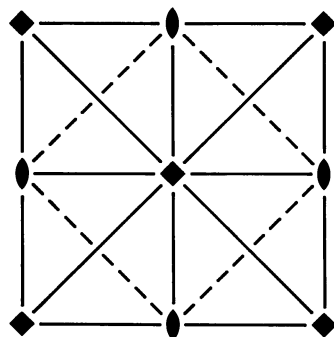
$4mm$

Tetragonal

No. 99

$P4mm$

Patterson symmetry $P4/mmm$



Origin on $4mm$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $x \leq y$

Symmetry operations

- | | | | |
|-----------------|-----------------|-----------------------|-------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) m $x,0,z$ | (6) m $0,y,z$ | (7) m x,\bar{x},z | (8) m x,x,z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>g</i> 1	(1) x, y, z (5) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z	(3) \bar{y}, x, z (7) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) y, x, z	General: no conditions Special: no extra conditions
4 <i>f</i> . <i>m</i> .	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$	$\frac{1}{2}, x, z$	$\frac{1}{2}, \bar{x}, z$	no extra conditions
4 <i>e</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z$	$0, \bar{x}, z$	no extra conditions
4 <i>d</i> . . <i>m</i>	x, x, z	\bar{x}, \bar{x}, z	\bar{x}, x, z	x, \bar{x}, z	no extra conditions
2 <i>c</i> 2 <i>m m</i> .	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$			$hkl : h + k = 2n$
1 <i>b</i> 4 <i>m m</i>	$\frac{1}{2}, \frac{1}{2}, z$				no extra conditions
1 <i>a</i> 4 <i>m m</i>	$0, 0, z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4, 75$) 1; 2; 3; 4
 [2] $P21m$ ($Cmm2, 35$) 1; 2; 7; 8
 [2] $P2m1$ ($Pmm2, 25$) 1; 2; 5; 6

IIa none

IIb [2] $P4_2mc$ ($\mathbf{c}' = 2\mathbf{c}$) (105); [2] $P4cc$ ($\mathbf{c}' = 2\mathbf{c}$) (103); [2] $P4_2cm$ ($\mathbf{c}' = 2\mathbf{c}$) (101); [2] $C4md$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4bm, 100$);
 [2] $F4mc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4cm, 108$); [2] $F4mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4mm, 107$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4mm$ ($\mathbf{c}' = 2\mathbf{c}$) (99); [2] $C4mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4mm, 99$)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

II [2] $I4mm$ (107)

$P4bm$

C_{4v}^2

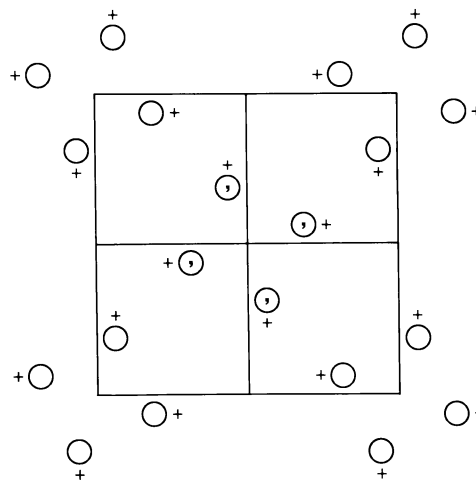
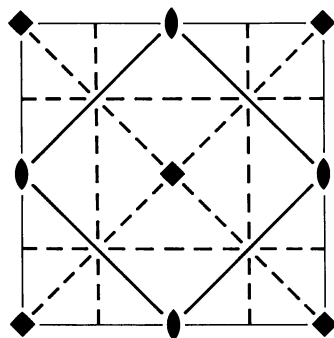
$4mm$

Tetragonal

No. 100

$P4bm$

Patterson symmetry $P4/mmm$



Origin on $41g$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $y \leq \frac{1}{2} - x$

Symmetry operations

- | | | | |
|-----------------------------|-----------------------------|---------------------------------------|--|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) a $x, \frac{1}{4}, z$ | (6) b $\frac{1}{4}, y, z$ | (7) m $x + \frac{1}{2}, \bar{x}, z$ | (8) $g(\frac{1}{2}, \frac{1}{2}, 0)$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>d</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{y}, x, z	(4) y, \bar{x}, z	$0kl : k = 2n$
	(5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(8) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$h00 : h = 2n$
					Special: as above, plus
4 <i>c</i> $\dots m$	$x, x + \frac{1}{2}, z$	$\bar{x}, \bar{x} + \frac{1}{2}, z$	$\bar{x} + \frac{1}{2}, x, z$	$x + \frac{1}{2}, \bar{x}, z$	no extra conditions
2 <i>b</i> $2 \dots mm$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$			$hkl : h + k = 2n$
2 <i>a</i> $4 \dots$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
 [2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
 [2] $P2b1$ ($Pba2$, 32) 1; 2; 5; 6

IIa none

IIb [2] $P4_2bc$ ($c' = 2c$) (106); [2] $P4nc$ ($c' = 2c$) (104); [2] $P4_2nm$ ($c' = 2c$) (102)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4bm$ ($c' = 2c$) (100); [9] $P4bm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (100)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/mbm$ (127)
II [2] $C4mm$ ($P4mm$, 99); [2] $I4cm$ (108)

$P4_2cm$

C_{4v}^3

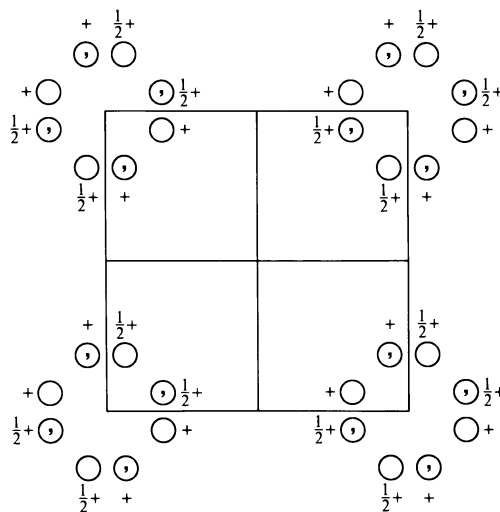
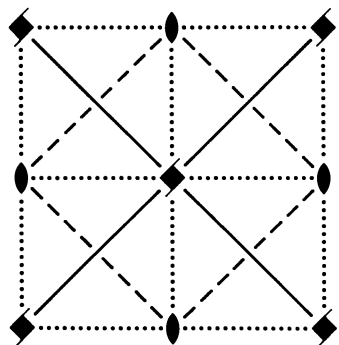
$4mm$

Tetragonal

No. 101

$P4_2cm$

Patterson symmetry $P4/mmm$



Origin on $2mm$ on 4_2cm

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $x \leq y$

Symmetry operations

- | | | | |
|-----------------|-----------------|------------------------------------|------------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ | (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$ |
| (5) c $x,0,z$ | (6) c $0,y,z$ | (7) m x,\bar{x},z | (8) m x,x,z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>e</i> 1	(1) x, y, z (5) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) \bar{y}, \bar{x}, z	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) y, x, z	General: $0kl : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
4 <i>d</i> $\dots m$	x, x, z	\bar{x}, \bar{x}, z	$\bar{x}, x, z + \frac{1}{2}$	$x, \bar{x}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>c</i> $2 \dots$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, z$	$hkl : l = 2n$
2 <i>b</i> $2 \dots mm$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			$hkl : l = 2n$
2 <i>a</i> $2 \dots mm$	$0, 0, z$	$0, 0, z + \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2, 77$) 1; 2; 3; 4
[2] $P21m$ ($Cmm2, 35$) 1; 2; 7; 8
[2] $P2c1$ ($Pcc2, 27$) 1; 2; 5; 6

IIa none

IIb [2] $C4_2cd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2bc, 106$); [2] $C4_2cm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2mc, 105$)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2cm$ ($\mathbf{c}' = 3\mathbf{c}$) (101); [9] $P4_2cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (101)

Minimal non-isomorphic supergroups

I [2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)

II [2] $C4_2cm$ ($P4_2mc, 105$); [2] $I4cm$ (108); [2] $P4mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (99)

$P4_2nm$

C_{4v}^4

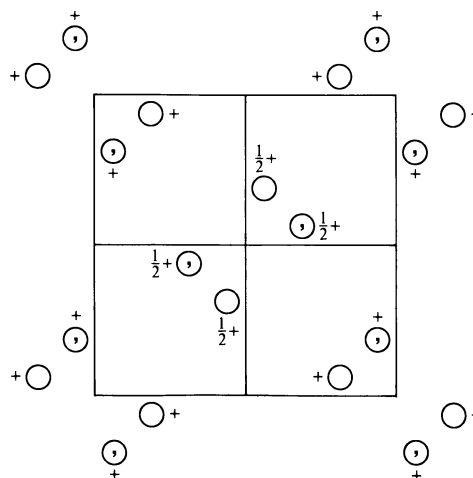
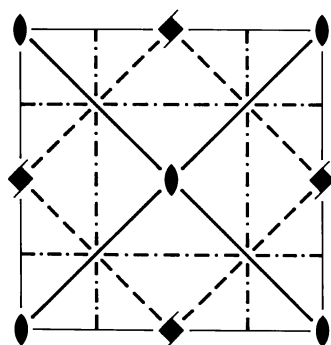
$4mm$

Tetragonal

No. 102

$P4_2nm$

Patterson symmetry $P4/mmm$



Origin on $2mm$ on $21m$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1; x \leq y$

Symmetry operations

- | | | | |
|--|--|--|--|
| (1) 1 | (2) $2 \quad 0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2}) \quad 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \quad \frac{1}{2}, 0, z$ |
| (5) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{4}, z$ | (6) $n(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{4}, y, z$ | (7) $m \quad x, \bar{x}, z$ | (8) $m \quad x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>d</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	$0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
	(5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	(7) \bar{y}, \bar{x}, z	(8) y, x, z	Special: as above, plus
4 <i>c</i> $\dots m$	x, x, z	\bar{x}, \bar{x}, z	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	no extra conditions
4 <i>b</i> $2 \dots$	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$\frac{1}{2}, 0, z$	$hkl : h + k, l = 2n$
2 <i>a</i> $2 \dots mm$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, \frac{1}{2}, z$

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_211 (P4_2, 77)$ 1; 2; 3; 4
 [2] $P21m (Cmm2, 35)$ 1; 2; 7; 8
 [2] $P2n1 (Pnn2, 34)$ 1; 2; 5; 6

IIa none

IIb [2] $F4_1dc (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I4_1cd, 110)$; [2] $F4_1dm (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (I4_1md, 109)$

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2nm (\mathbf{c}' = 3\mathbf{c}) (102)$; [9] $P4_2nm (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (102)$

Minimal non-isomorphic supergroups

I [2] $P4_2/nnm (134)$; [2] $P4_2/mnm (136)$

II [2] $C4_2cm (P4_2mc, 105)$; [2] $I4mm (107)$; [2] $P4bm (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (100)$

$P4cc$

C_{4v}^5

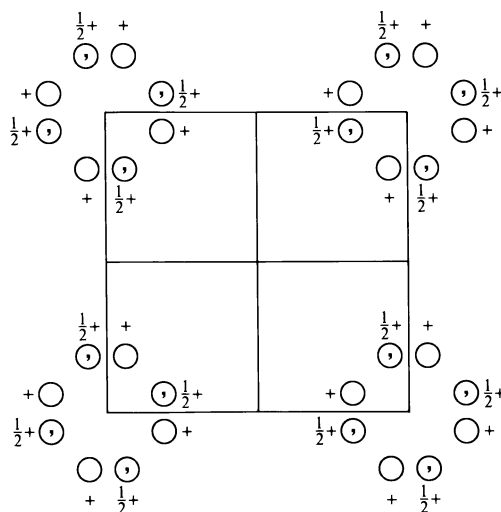
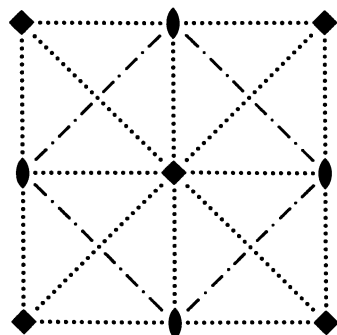
$4mm$

Tetragonal

No. 103

$P4cc$

Patterson symmetry $P4/mmm$



Origin on $4c$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------|-----------------|-----------------------|-------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) c $x,0,z$ | (6) c $0,y,z$ | (7) c x,\bar{x},z | (8) c x,x,z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>d</i> 1	(1) x, y, z (5) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $\bar{x}, y, z + \frac{1}{2}$	(3) \bar{y}, x, z (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) y, \bar{x}, z (8) $y, x, z + \frac{1}{2}$	General: $0kl : l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : h + k, l = 2n$ $hkl : l = 2n$ $hkl : l = 2n$
4 <i>c</i> 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	
2 <i>b</i> 4..	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			
2 <i>a</i> 4..	$0, 0, z$	$0, 0, z + \frac{1}{2}$			

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p1m1$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p1m1$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4, 75$) 1; 2; 3; 4

[2] $P21c$ ($Ccc2, 37$) 1; 2; 7; 8

[2] $P2c1$ ($Pcc2, 27$) 1; 2; 5; 6

IIa none

IIb [2] $C4cd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4nc, 104$)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4cc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4cc, 103$); [3] $P4cc$ ($\mathbf{c}' = 3\mathbf{c}$) (103)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4/ncc$ (130)

II [2] $I4cm$ (108); [2] $P4mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (99)

$P4nc$

C_{4v}^6

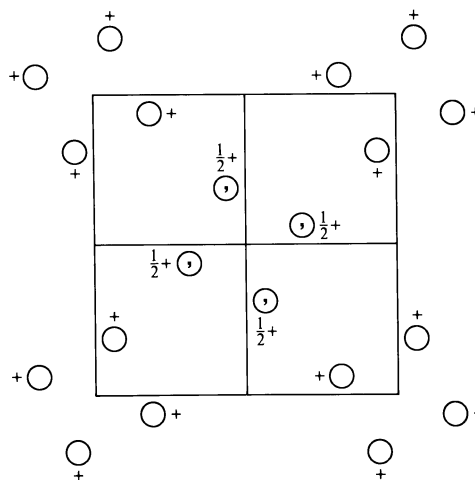
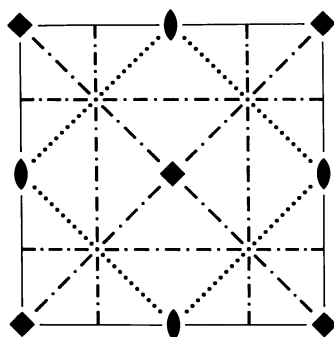
$4mm$

Tetragonal

No. 104

$P4nc$

Patterson symmetry $P4/mmm$



Origin on $41n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|--|--|---|--|
| (1) 1 | (2) $2 \quad 0, 0, z$ | (3) $4^+ \quad 0, 0, z$ | (4) $4^- \quad 0, 0, z$ |
| (5) $n(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{4}, z$ | (6) $n(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{4}, y, z$ | (7) $c \quad x + \frac{1}{2}, \bar{x}, z$ | (8) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>c</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{y}, x, z	(4) y, \bar{x}, z	$0kl : k + l = 2n$
	(5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	(7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(8) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hhl : l = 2n$
					$00l : l = 2n$
					$h00 : h = 2n$
					Special: as above, plus
4 <i>b</i> 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
2 <i>a</i> 4..	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4, 75$) 1; 2; 3; 4
 [2] $P21c$ ($Ccc2, 37$) 1; 2; 7; 8
 [2] $P2n1$ ($Pnn2, 34$) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4nc$ ($\mathbf{c}' = 3\mathbf{c}$) (104); [9] $P4nc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (104)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4/mnc$ (128)

II [2] $C4cc$ ($P4cc, 103$); [2] $I4mm$ (107); [2] $P4bm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (100)

$P4_2mc$

C_{4v}^7

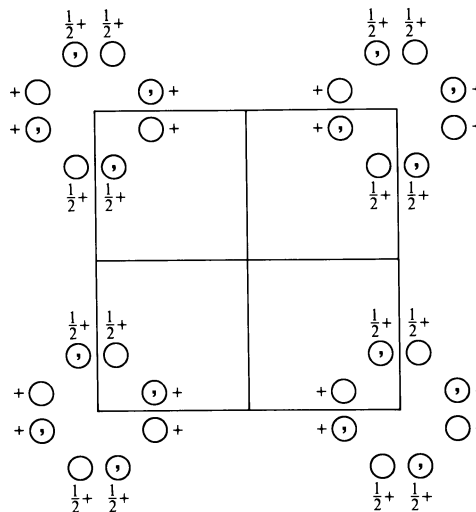
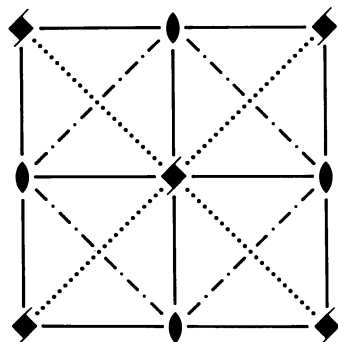
$4mm$

Tetragonal

No. 105

$P4_2mc$

Patterson symmetry $P4/mmm$



Origin on $2mm$ on 4_2mc

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------|-------------------|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, 0, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $0, 0, z$ |
| (5) m $x, 0, z$ | (6) m $0, y, z$ | (7) c x, \bar{x}, z | (8) c x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>f</i> 1	(1) x, y, z (5) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $y, x, z + \frac{1}{2}$	General: $hkl : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
4 <i>e</i> . <i>m</i> .	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$	$\frac{1}{2}, x, z + \frac{1}{2}$	$\frac{1}{2}, \bar{x}, z + \frac{1}{2}$	no extra conditions
4 <i>d</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z + \frac{1}{2}$	$0, \bar{x}, z + \frac{1}{2}$	no extra conditions
2 <i>c</i> 2 <i>m</i> <i>m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$			$hkl : h + k + l = 2n$
2 <i>b</i> 2 <i>m</i> <i>m</i> .	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$			$hkl : l = 2n$
2 <i>a</i> 2 <i>m</i> <i>m</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[110]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2, 77$) 1; 2; 3; 4
[2] $P21c$ ($Ccc2, 37$) 1; 2; 7; 8
[2] $P2m1$ ($Pmm2, 25$) 1; 2; 5; 6

IIa none

IIb [2] $C4_2md$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2nm, 102$); [2] $C4_2mc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2cm, 101$)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2mc$ ($\mathbf{c}' = 3\mathbf{c}$) (105); [9] $P4_2mc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (105)

Minimal non-isomorphic supergroups

I [2] $P4_2/mmc$ (131); [2] $P4_2/nmc$ (137)

II [2] $C4_2mc$ ($P4_2cm, 101$); [2] $I4mm$ (107); [2] $P4mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (99)

$P4_2bc$

C_{4v}^8

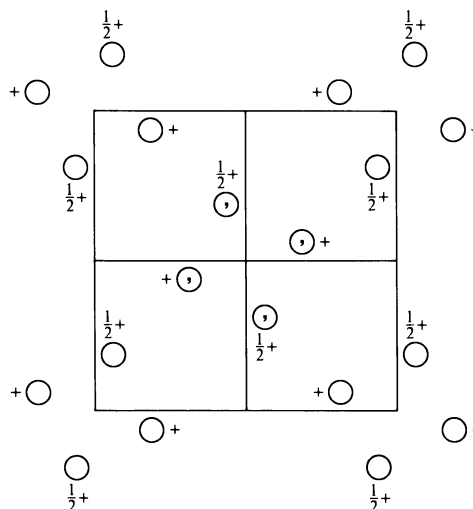
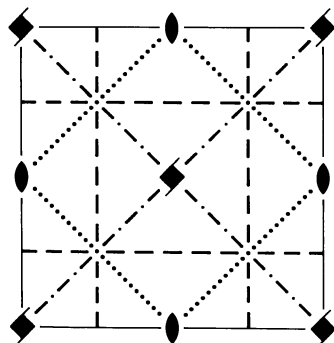
$4mm$

Tetragonal

No. 106

$P4_2bc$

Patterson symmetry $P4/mmm$



Origin on 2 on $4_2 1n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---------------------------|---------------------------|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, 0, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $0, 0, z$ |
| (5) a $x, \frac{1}{4}, z$ | (6) b $\frac{1}{4}, y, z$ | (7) c $x + \frac{1}{2}, \bar{x}, z$ | (8) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>c</i> 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{y}, x, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$	General: $0kl : k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus $hkl : h + k, l = 2n$ $hkl : h + k, l = 2n$
	(5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(8) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	
4 <i>b</i> 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>a</i> 2..	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2, 77$) 1; 2; 3; 4
 [2] $P21c$ ($Ccc2, 37$) 1; 2; 7; 8
 [2] $P2b1$ ($Pba2, 32$) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2bc$ ($\mathbf{c}' = 3\mathbf{c}$) (106); [9] $P4_2bc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (106)

Minimal non-isomorphic supergroups

I [2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

II [2] $C4_2mc$ ($P4_2cm, 101$); [2] $I4cm$ (108); [2] $P4bm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (100)

$I4mm$

C_{4v}^9

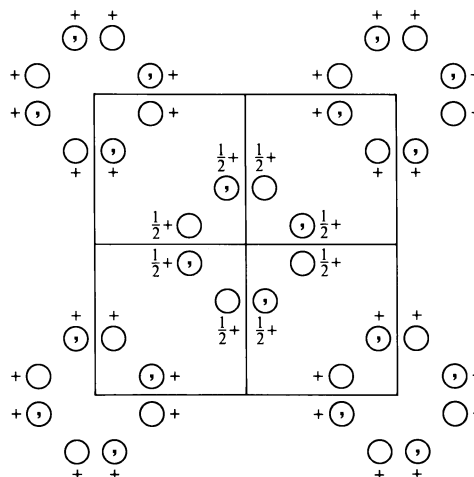
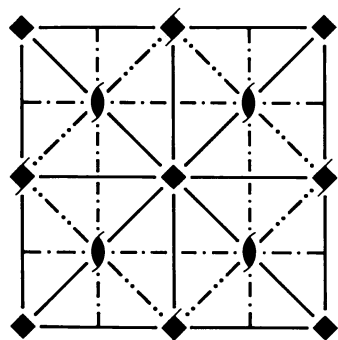
$4mm$

Tetragonal

No. 107

$I4mm$

Patterson symmetry $I4/mmm$



Origin on $4mm$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $x \leq y$

Symmetry operations

For $(0,0,0)^+$ set

- | | | | |
|----------------|----------------|----------------------|-----------------|
| (1) 1 | (2) $2\ 0,0,z$ | (3) $4^+ 0,0,z$ | (4) $4^- 0,0,z$ |
| (5) $m\ x,0,z$ | (6) $m\ 0,y,z$ | (7) $m\ x,\bar{x},z$ | (8) $m\ x,x,z$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})^+$ set

- | | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})\ \frac{1}{4},\frac{1}{4},z$ | (3) $4^+(0,0,\frac{1}{2})\ 0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{2})\ \frac{1}{2},0,z$ |
| (5) $n(\frac{1}{2},0,\frac{1}{2})\ x,\frac{1}{4},z$ | (6) $n(0,\frac{1}{2},\frac{1}{2})\ \frac{1}{4},y,z$ | (7) $c\ x+\frac{1}{2},\bar{x},z$ | (8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ x,x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16 <i>e</i> 1	(1) x, y, z (5) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z	(3) \bar{y}, x, z (7) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) y, x, z		$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$
8 <i>d</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z$	$0, \bar{x}, z$		Special: as above, plus no extra conditions
8 <i>c</i> . <i>.</i> <i>m</i>	x, x, z	\bar{x}, \bar{x}, z	\bar{x}, x, z	x, \bar{x}, z		no extra conditions
4 <i>b</i> 2 <i>m</i> <i>m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$				$hkl : l=2n$
2 <i>a</i> 4 <i>m</i> <i>m</i>	$0, 0, z$					no extra conditions

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $c1m1$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I411$ ($I4, 79$)	(1; 2; 3; 4)+
	[2] $I2m1$ ($Imm2, 44$)	(1; 2; 5; 6)+
	[2] $I21m$ ($Fmm2, 42$)	(1; 2; 7; 8)+
IIa	[2] $P4_2mc$ (105)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4nc$ (104)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2nm$ (102)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4mm$ (99)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4mm$ ($\mathbf{c}' = 3\mathbf{c}$) (107); [9] $I4mm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (107)

Minimal non-isomorphic supergroups

I	[2] $I4/mmm$ (139)
II	[2] $C4mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4mm, 99$)

$I4cm$

C_{4v}^{10}

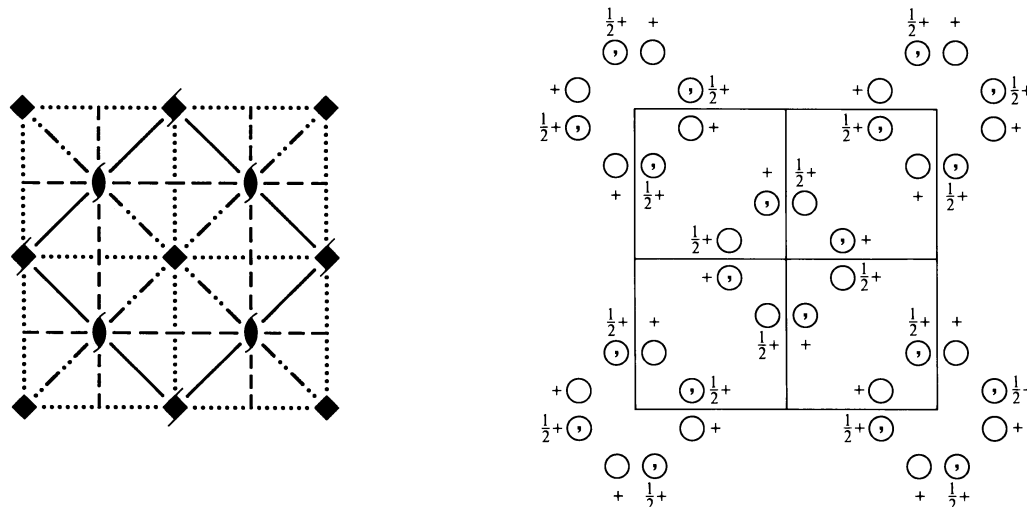
$4mm$

Tetragonal

No. 108

$I4cm$

Patterson symmetry $I4/mmm$



Origin on $4c$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \frac{1}{2} - x$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|----------------|----------------|----------------------|-----------------|
| (1) 1 | (2) $2\ 0,0,z$ | (3) $4^+ 0,0,z$ | (4) $4^- 0,0,z$ |
| (5) $c\ x,0,z$ | (6) $c\ 0,y,z$ | (7) $c\ x,\bar{x},z$ | (8) $c\ x,x,z$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- | | | | |
|--|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})\ \frac{1}{4},\frac{1}{4},z$ | (3) $4^+(0,0,\frac{1}{2})\ 0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{2})\ \frac{1}{2},0,z$ |
| (5) $a\ x,\frac{1}{4},z$ | (6) $b\ \frac{1}{4},y,z$ | (7) $m\ x+\frac{1}{2},\bar{x},z$ | (8) $g(\frac{1}{2},\frac{1}{2},0)\ x,x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ +				General:
16 <i>d</i> 1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) \bar{x},\bar{y},z (6) $\bar{x},y,z+\frac{1}{2}$	(3) \bar{y},x,z (7) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) y,\bar{x},z (8) $y,x,z+\frac{1}{2}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k,l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$
8 <i>c</i> . . <i>m</i>	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	Special: as above, plus no extra conditions
4 <i>b</i> 2 . <i>mm</i>	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			$hkl : l=2n$
4 <i>a</i> 4 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			$hkl : l=2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0,0,z

Along [100] $p1m1$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at x,0,0

Along [110] $p1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at x,x,0

Maximal non-isomorphic subgroups

I	[2] $I411$ ($I4, 79$)	(1; 2; 3; 4)+
	[2] $I2c1$ ($Iba2, 45$)	(1; 2; 5; 6)+
	[2] $I21m$ ($Fmm2, 42$)	(1; 2; 7; 8)+
IIa	[2] $P4_2bc$ (106)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4cc$ (103)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2cm$ (101)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4bm$ (100)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4cm$ ($\mathbf{c}' = 3\mathbf{c}$) (108); [9] $I4cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (108)

Minimal non-isomorphic supergroups

I	[2] $I4/mcm$ (140)
II	[2] $C4mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4mm, 99$)

$I4_1md$

C_{4v}^{11}

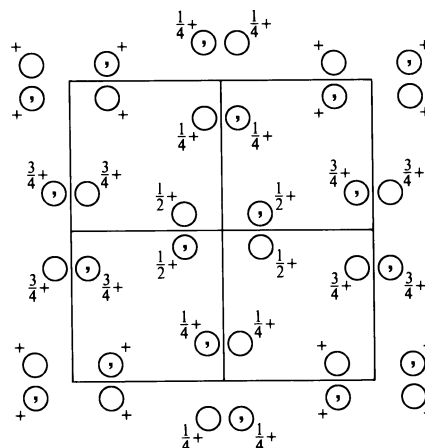
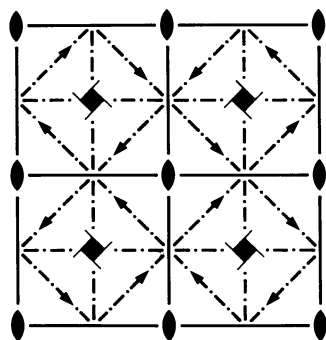
$4mm$

Tetragonal

No. 109

$I4_1md$

Patterson symmetry $I4/mmm$



Origin on $2mm$ on $2m1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------|--|---|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ | (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$ | (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$ |
| (5) m $x,0,z$ | (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ | (7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$ | (8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- | | | | |
|--|-----------------|---|--|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) 2 $0,0,z$ | (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$ | (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$ |
| (5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ | (6) m $0,y,z$ | (7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$ | (8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16 <i>c</i> 1	(1) x, y, z (5) x, \bar{y}, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (7) $\bar{y}, \bar{x} + \frac{1}{2}, z + \frac{1}{4}$	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (8) $y + \frac{1}{2}, x, z + \frac{3}{4}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
8 <i>b</i> . <i>m</i> .	$0, y, z$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	$\bar{y}, \frac{1}{2}, z + \frac{1}{4}$	$y + \frac{1}{2}, 0, z + \frac{3}{4}$	Special: as above, plus no extra conditions
4 <i>a</i> 2 <i>m</i> <i>m</i> .	$0, 0, z$	$0, \frac{1}{2}, z + \frac{1}{4}$			$hkl : l = 2n + 1$ or $2h + l = 4n$

Symmetry of special projections

Along [001] $p4gm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $c1m1$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $c1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I4_1 11 (I4_1, 80)$	(1; 2; 3; 4)+
	[2] $I2m1 (Imm2, 44)$	(1; 2; 5; 6)+
	[2] $I21d (Fdd2, 43)$	(1; 2; 7; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1md (\mathbf{c}' = 3\mathbf{c}) (109)$; [9] $I4_1md (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (109)$

Minimal non-isomorphic supergroups

I [2] $I4_1/amd (141)$

II [2] $C4_2md (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (P4_2nm, 102)$

$I4_1cd$

C_{4v}^{12}

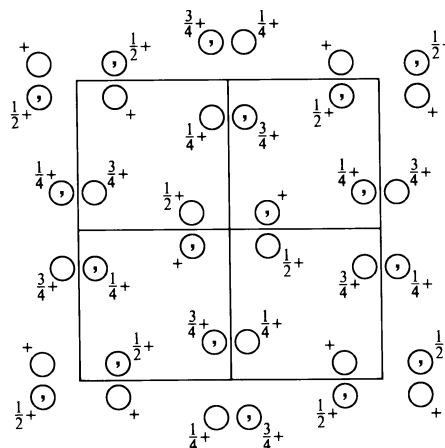
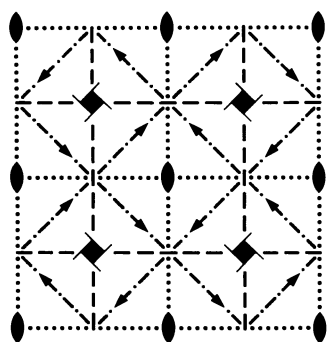
$4mm$

Tetragonal

No. 110

$I4_1cd$

Patterson symmetry $I4/mmm$



Origin on $2c1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------------|--|---|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{1}{4}) \quad -\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{3}{4}) \quad \frac{1}{4}, -\frac{1}{4}, z$ |
| (5) $c \quad x, 0, z$ | (6) $b \quad \frac{1}{4}, y, z$ | (7) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4}) \quad x + \frac{1}{4}, \bar{x}, z$ | (8) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) \quad x + \frac{1}{4}, x, z$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--|-----------------------|---|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, 0, z$ | (3) $4^+(0,0,\frac{3}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{1}{4}) \quad \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $a \quad x, \frac{1}{4}, z$ | (6) $c \quad 0, y, z$ | (7) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}) \quad x + \frac{1}{4}, \bar{x}, z$ | (8) $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}) \quad x - \frac{1}{4}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	General:
16 <i>b</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (5) $x, \bar{y}, z + \frac{1}{2}$ (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (7) $\bar{y}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$ (8) $y + \frac{1}{2}, x, z + \frac{1}{4}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k, l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
8 <i>a</i> 2..	$0, 0, z$ $0, \frac{1}{2}, z + \frac{1}{4}$ $0, 0, z + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{3}{4}$	Special: as above, plus $hkl : 2h + l = 4n$

Symmetry of special projections

Along $[001]$ $p4gm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along $[100]$ $p1m1$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, 0, 0$

Along $[110]$ $c1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** [2] $I4_111$ ($I4_1, 80$) (1; 2; 3; 4)+
 [2] $I2c1$ ($Iba2, 45$) (1; 2; 5; 6)+
 [2] $I21d$ ($Fdd2, 43$) (1; 2; 7; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1cd$ ($\mathbf{c}' = 3\mathbf{c}$) (110); [9] $I4_1cd$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (110)

Minimal non-isomorphic supergroups

I [2] $I4_1/acd$ (142)

II [2] $C4_2md$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4_2nm, 102$)

$P\bar{4}2m$

D_{2d}^1

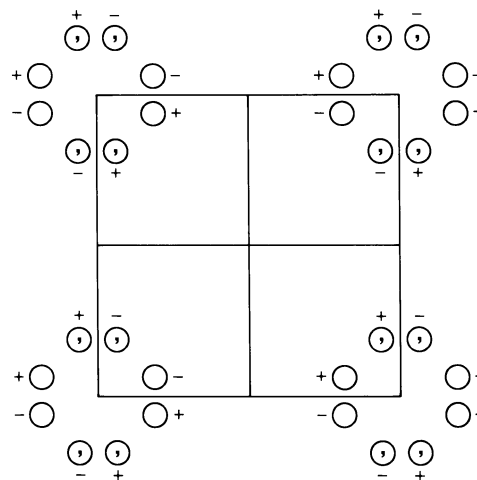
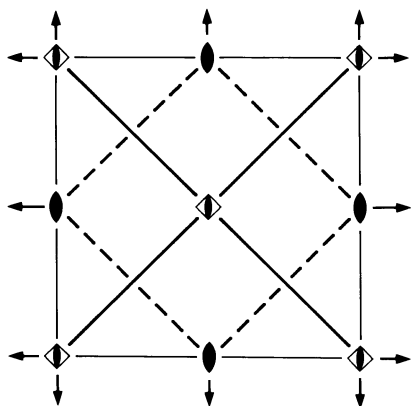
$\bar{4}2m$

Tetragonal

No. 111

$P\bar{4}2m$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}2m$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $x \leq y$

Symmetry operations

- | | | | |
|---------------|---------------|-----------------------------------|-----------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ | (4) $\bar{4}^-$ $0,0,z$; $0,0,0$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) m x,\bar{x},z | (8) m x,x,z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>o</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z}	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z}	(3) y, \bar{x}, \bar{z} (7) \bar{y}, \bar{x}, z	(4) \bar{y}, x, \bar{z} (8) y, x, z	General: no conditions Special:
4 <i>n</i> . . <i>m</i>	x, x, z	\bar{x}, \bar{x}, z	x, \bar{x}, \bar{z}	\bar{x}, x, \bar{z}	no extra conditions
4 <i>m</i> 2 . .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$	$hkl : h + k = 2n$
4 <i>l</i> . 2 .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, \bar{x}, 0$	$\frac{1}{2}, x, 0$	no extra conditions
4 <i>k</i> . 2 .	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$0, x, \frac{1}{2}$	no extra conditions
4 <i>j</i> . 2 .	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	no extra conditions
4 <i>i</i> . 2 .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$0, x, 0$	no extra conditions
2 <i>h</i> 2 . <i>mm</i>	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions
2 <i>g</i> 2 . <i>mm</i>	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
2 <i>f</i> 2 2 2 .	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>e</i> 2 2 2 .	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$			$hkl : h + k = 2n$
1 <i>d</i> $\bar{4}2m$	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
1 <i>c</i> $\bar{4}2m$	$0, 0, \frac{1}{2}$				no extra conditions
1 <i>b</i> $\bar{4}2m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				no extra conditions
1 <i>a</i> $\bar{4}2m$	$0, 0, 0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p1m1$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}11$ ($P\bar{4}$, 81)	1; 2; 3; 4
	[2] $P21m$ ($Cmm2$, 35)	1; 2; 7; 8
	[2] $P221$ ($P222$, 16)	1; 2; 5; 6

IIa none

IIb [2] $P\bar{4}2c$ ($\mathbf{c}' = 2\mathbf{c}$) (112); [2] $C\bar{4}2d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}b2$, 117); [2] $C\bar{4}2m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}m2$, 115);
[2] $F\bar{4}2c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}c2$, 120); [2] $F\bar{4}2m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}m2$, 119)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}2m$ ($\mathbf{c}' = 2\mathbf{c}$) (111); [9] $P\bar{4}2m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (111)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/nbm$ (125); [2] $P4_2/mcm$ (132); [2] $P4_2/nnm$ (134); [3] $P\bar{4}3m$ (215)

II [2] $C\bar{4}2m$ ($P\bar{4}m2$, 115); [2] $I\bar{4}2m$ (121)

$P\bar{4}2c$

D_{2d}^2

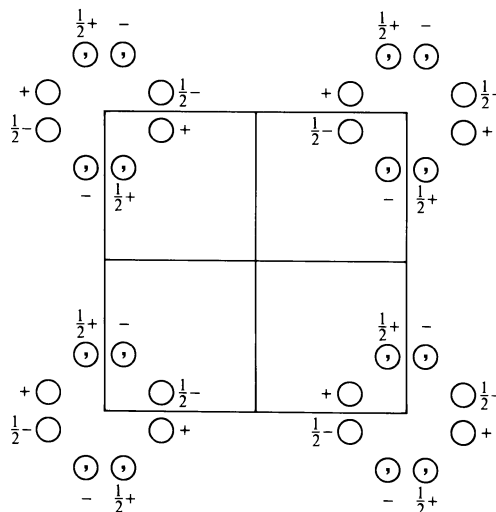
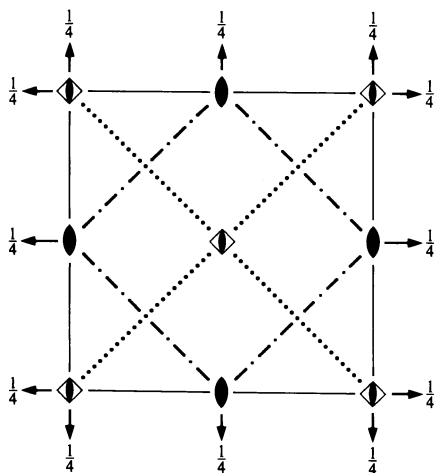
$\bar{4}2m$

Tetragonal

No. 112

$P\bar{4}2c$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}1c$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---------------------------|---------------------------|----------------------------------|----------------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $\bar{4}^+ 0, 0, z; 0, 0, 0$ | (4) $\bar{4}^- 0, 0, z; 0, 0, 0$ |
| (5) 2 $0, y, \frac{1}{4}$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) c x, \bar{x}, z | (8) c x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>n</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (3) y, \bar{x}, \bar{z} (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (4) \bar{y}, x, \bar{z} (8) $y, x, z + \frac{1}{2}$	General: $hkl : l = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>m</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>l</i> 2..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>k</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$ $0, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>j</i> .2.	$0, y, \frac{1}{4}$ $0, \bar{y}, \frac{1}{4}$ $y, 0, \frac{3}{4}$ $\bar{y}, 0, \frac{3}{4}$	no extra conditions
4 <i>i</i> .2.	$x, \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \bar{x}, \frac{3}{4}$ $\frac{1}{2}, x, \frac{3}{4}$	no extra conditions
4 <i>h</i> .2.	$\frac{1}{2}, y, \frac{1}{4}$ $\frac{1}{2}, \bar{y}, \frac{1}{4}$ $y, \frac{1}{2}, \frac{3}{4}$ $\bar{y}, \frac{1}{2}, \frac{3}{4}$	no extra conditions
4 <i>g</i> .2.	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$ $0, x, \frac{3}{4}$	no extra conditions
2 <i>f</i> $\bar{4}$..	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n$
2 <i>e</i> $\bar{4}$..	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : l = 2n$
2 <i>d</i> 222.	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>c</i> 222.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : l = 2n$
2 <i>b</i> 222.	$\frac{1}{2}, 0, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> 222.	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, \frac{1}{4}$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P221$ ($P222$, 16) 1; 2; 5; 6

IIa none

IIb [2] $C\bar{4}2d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}n2$, 118); [2] $C\bar{4}2c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}c2$, 116)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}2c$ ($\mathbf{c}' = 3\mathbf{c}$) (112); [9] $P\bar{4}2c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (112)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4/nnc$ (126); [2] $P4_2/mmc$ (131); [2] $P4_2/nbc$ (133); [3] $P\bar{4}3n$ (218)

II [2] $C\bar{4}2c$ ($P\bar{4}c2$, 116); [2] $I\bar{4}2m$ (121); [2] $P\bar{4}2m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (111)

$P\bar{4}2_1m$

D_{2d}^3

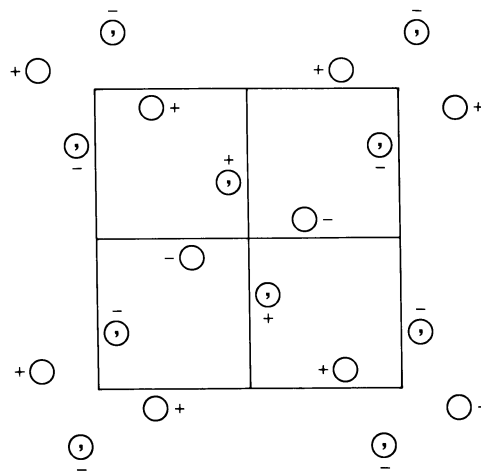
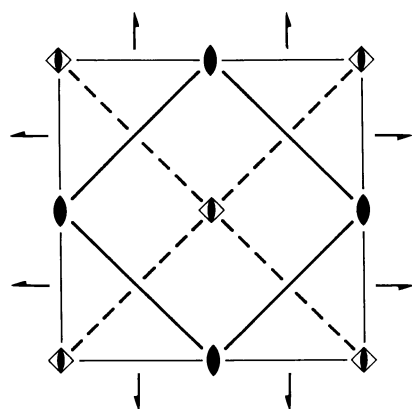
$\bar{4}2m$

Tetragonal

No. 113

$P\bar{4}2_1m$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}1g$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1; y \leq \frac{1}{2} - x$

Symmetry operations

- | | | | |
|--|--|---|--|
| (1) 1 | (2) $2 \quad 0, 0, z$ | (3) $\bar{4}^+ \quad 0, 0, z; 0, 0, 0$ | (4) $\bar{4}^- \quad 0, 0, z; 0, 0, 0$ |
| (5) $2(0, \frac{1}{2}, 0) \quad \frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ | (7) $m \quad x + \frac{1}{2}, \bar{x}, z$ | (8) $g(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>f</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(3) y, \bar{x}, \bar{z} (7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) \bar{y}, x, \bar{z} (8) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk0 : h = 2n$ Special: as above, plus no extra conditions
4 <i>e</i> $\dots m$	$x, x + \frac{1}{2}, z$	$\bar{x}, \bar{x} + \frac{1}{2}, z$	$x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, \bar{z}$	$hkl : h + k = 2n$
4 <i>d</i> $2 \dots$	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hk0 : h + k = 2n$
2 <i>c</i> $2 \dots mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			$hkl : h + k = 2n$
2 <i>b</i> $\bar{4} \dots$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> $\bar{4} \dots$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along $[001]$ $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, 0$

Along $[110]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I $[2] P\bar{4}11 (P\bar{4}, 81)$ 1; 2; 3; 4
 $[2] P21m (Cmm2, 35)$ 1; 2; 7; 8
 $[2] P22_11 (P2_12_12, 18)$ 1; 2; 5; 6

IIa none

IIb $[2] P\bar{4}2_1c (c' = 2c) (114)$

Maximal isomorphic subgroups of lowest index

IIc $[2] P\bar{4}2_1m (c' = 2c) (113)$; $[9] P\bar{4}2_1m (a' = 3a, b' = 3b) (113)$

Minimal non-isomorphic supergroups

I $[2] P4/mbm (127)$; $[2] P4/nmm (129)$; $[2] P4_2/mnm (136)$; $[2] P4_2/ncm (138)$

II $[2] C\bar{4}2m (P\bar{4}m2, 115)$; $[2] I\bar{4}2m (121)$

$P\bar{4}2_1c$

D_{2d}^4

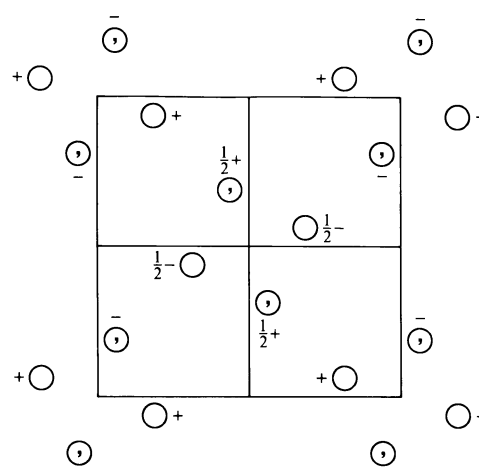
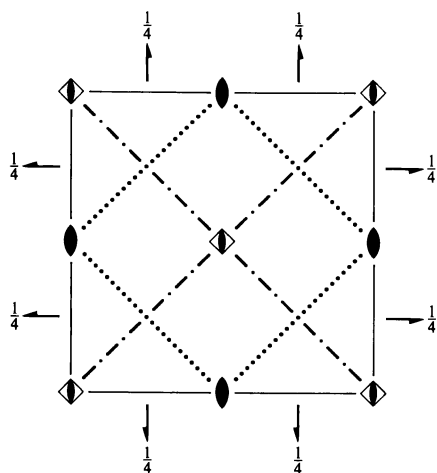
$\bar{4}2m$

Tetragonal

No. 114

$P\bar{4}2_1c$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}1n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|--|--|---------------------------------------|--|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $\bar{4}^+ \ 0,0,z; 0,0,0$ | (4) $\bar{4}^- \ 0,0,z; 0,0,0$ |
| (5) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, \frac{1}{4}$ | (7) $c \ x + \frac{1}{2}, \bar{x}, z$ | (8) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

	Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
						General:
8	e 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) y, \bar{x}, \bar{z} (7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(4) \bar{y}, x, \bar{z} (8) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
4	d 2..	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$ $hk0 : h + k = 2n$
4	c 2..	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
2	b $\bar{4}$..	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2	a $\bar{4}$..	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mg$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [110] $p1m1$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}11$ ($P\bar{4}$, 81)	1; 2; 3; 4
	[2] $P21c$ ($Ccc2$, 37)	1; 2; 7; 8
	[2] $P22_11$ ($P2_12_12$, 18)	1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}2_1c$ ($\mathbf{c}' = 3\mathbf{c}$) (114); [9] $P\bar{4}2_1c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (114)

Minimal non-isomorphic supergroups

I [2] $P4/mnc$ (128); [2] $P4/ncc$ (130); [2] $P4_2/mbc$ (135); [2] $P4_2/nmc$ (137)

II [2] $C\bar{4}2c$ ($P\bar{4}c2$, 116); [2] $I\bar{4}2m$ (121); [2] $P\bar{4}2_1m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (113)

$P\bar{4}m2$

D_{2d}^5

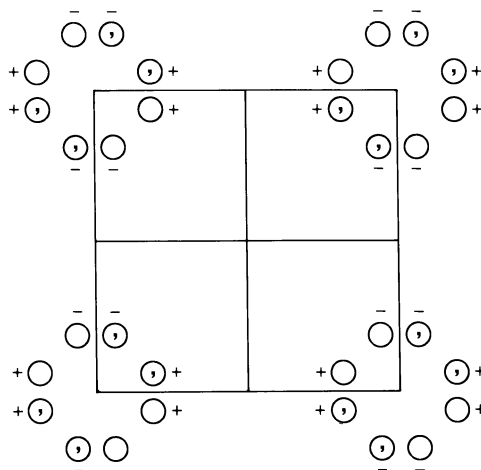
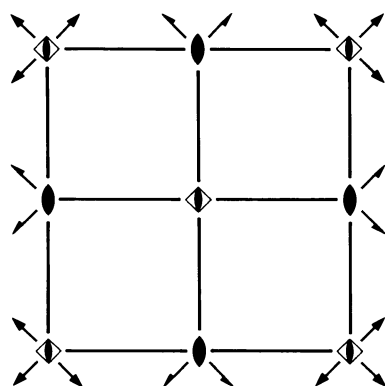
$\bar{4}m2$

Tetragonal

No. 115

$P\bar{4}m2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}m2$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------|-----------------|--------------------------------|--------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $\bar{4}^+$ $0,0,z; 0,0,0$ | (4) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (5) m $x,0,z$ | (6) m $0,y,z$ | (7) 2 $x,x,0$ | (8) 2 $x,\bar{x},0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>l</i> 1	(1) x, y, z (5) x, \bar{y}, z (2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z (3) y, \bar{x}, \bar{z} (7) y, x, \bar{z} (4) \bar{y}, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$	General: no conditions Special:
4 <i>k</i> . <i>m</i> .	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$ $\frac{1}{2}, x, \bar{z}$	no extra conditions
4 <i>j</i> . <i>m</i> .	$x, 0, z$ $\bar{x}, 0, z$ $0, \bar{x}, \bar{z}$ $0, x, \bar{z}$	no extra conditions
4 <i>i</i> . . 2	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $x, \bar{x}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$	no extra conditions
4 <i>h</i> . . 2	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $x, \bar{x}, 0$ $\bar{x}, x, 0$	no extra conditions
2 <i>g</i> 2 <i>m m</i> .	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$	$hk0 : h + k = 2n$
2 <i>f</i> 2 <i>m m</i> .	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
2 <i>e</i> 2 <i>m m</i> .	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
1 <i>d</i> $\bar{4}m2$	$0, 0, \frac{1}{2}$	no extra conditions
1 <i>c</i> $\bar{4}m2$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	no extra conditions
1 <i>b</i> $\bar{4}m2$	$\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions
1 <i>a</i> $\bar{4}m2$	$0, 0, 0$	no extra conditions

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2m1$ ($Pmm2$, 25) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $P\bar{4}c2$ ($\mathbf{c}' = 2\mathbf{c}$) (116); [2] $C\bar{4}m2_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}2_1m$, 113); [2] $C\bar{4}m2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}2m$, 111);
[2] $F\bar{4}m2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}2m$, 121)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}m2$ ($\mathbf{c}' = 2\mathbf{c}$) (115); [9] $P\bar{4}m2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (115)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129); [2] $P4_2/mmc$ (131); [2] $P4_2/nmc$ (137)
II [2] $C\bar{4}m2$ ($P\bar{4}2m$, 111); [2] $I\bar{4}m2$ (119)

$P\bar{4}c2$

D_{2d}^6

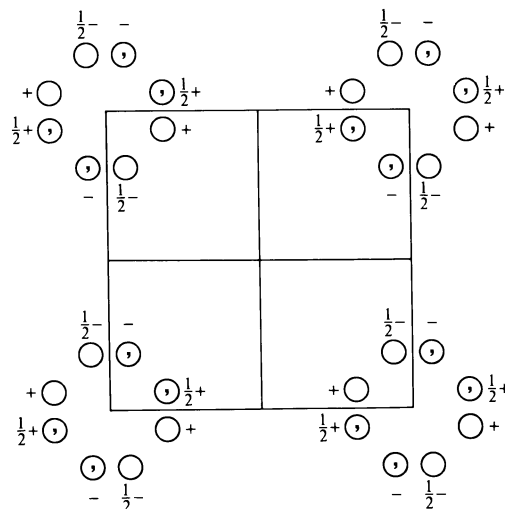
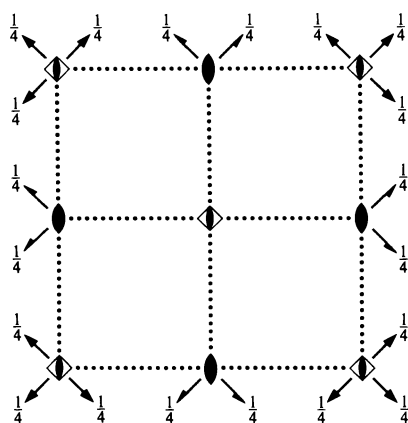
$\bar{4}m2$

Tetragonal

No. 116

$P\bar{4}c2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}c1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|-----------------|-----------------|-----------------------------------|-----------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ | (4) $\bar{4}^-$ $0,0,z$; $0,0,0$ |
| (5) c $x,0,z$ | (6) c $0,y,z$ | (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>j</i> 1	(1) x, y, z (5) $x, \bar{y}, z + \frac{1}{2}$ (2) \bar{x}, \bar{y}, z (6) $\bar{x}, y, z + \frac{1}{2}$ (3) y, \bar{x}, \bar{z} (7) $y, x, \bar{z} + \frac{1}{2}$ (4) \bar{y}, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	General: $0kl : l = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>i</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$ $hk0 : h + k = 2n$
4 <i>h</i> 2..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4 <i>g</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4 <i>f</i> ..2	$x, x, \frac{3}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$ $x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{1}{4}$	no extra conditions
4 <i>e</i> ..2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	no extra conditions
2 <i>d</i> $\bar{4}$..	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n$
2 <i>c</i> $\bar{4}$..	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : l = 2n$
2 <i>b</i> 2..22	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : l = 2n$
2 <i>a</i> 2..22	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p1m1$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
 [2] $P2c1$ ($Pcc2$, 27) 1; 2; 5; 6
 [2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $C\bar{4}c2_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}2_1c$, 114); [2] $C\bar{4}c2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}2c$, 112)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}c2$ ($\mathbf{c}' = 3\mathbf{c}$) (116); [9] $P\bar{4}c2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (116)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4/ncc$ (130); [2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)

II [2] $C\bar{4}c2$ ($P\bar{4}2c$, 112); [2] $I\bar{4}c2$ (120); [2] $P\bar{4}m2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (115)

$P\bar{4}b2$

D_{2d}^7

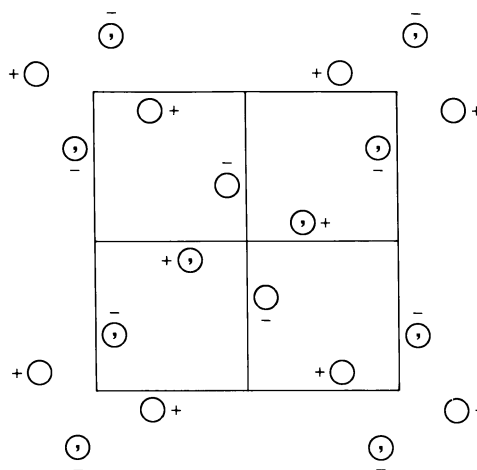
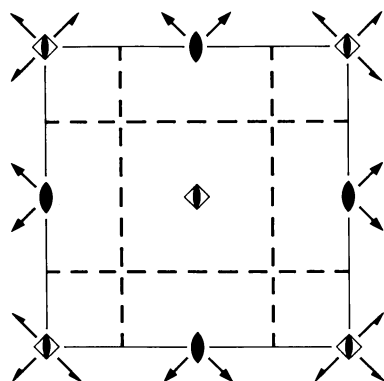
$\bar{4}m2$

Tetragonal

No. 117

$P\bar{4}b2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}12_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- | | | | |
|---------------------------|---------------------------|--|-------------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $\bar{4}^+ 0,0,z; 0,0,0$ | (4) $\bar{4}^- 0,0,z; 0,0,0$ |
| (5) a $x, \frac{1}{4}, z$ | (6) b $\frac{1}{4}, y, z$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>i</i> 1	(1) x, y, z (5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) \bar{x}, \bar{y}, z (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$
	(3) y, \bar{x}, \bar{z} (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(4) \bar{y}, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$
		General: $Ok\bar{l} : k = 2n$ $h00 : h = 2n$
		Special: as above, plus
4 <i>h</i> ..2	$x, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$	no extra conditions
4 <i>g</i> ..2	$x, x + \frac{1}{2}, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x, 0$	no extra conditions
4 <i>f</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$	$hkl : h + k = 2n$
4 <i>e</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	$hkl : h + k = 2n$
2 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>c</i> 2.22	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : h + k = 2n$
2 <i>b</i> $\bar{4}$..	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>a</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
 [2] $P2b1$ ($Pba2$, 32) 1; 2; 5; 6
 [2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $P\bar{4}n2$ ($\mathbf{c}' = 2\mathbf{c}$) (118)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}b2$ ($\mathbf{c}' = 2\mathbf{c}$) (117); [9] $P\bar{4}b2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (117)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/mbm$ (127); [2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

II [2] $C\bar{4}m2$ ($P\bar{4}2m$, 111); [2] $I\bar{4}c2$ (120)

$P\bar{4}n2$

D_{2d}^8

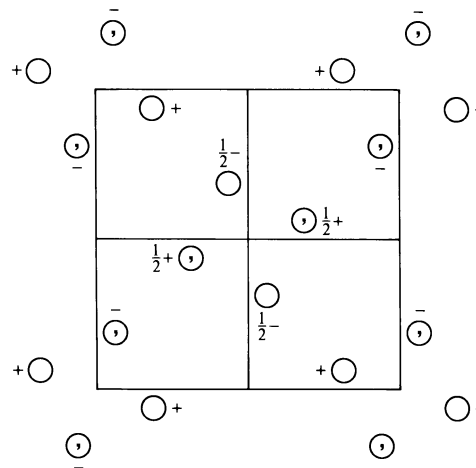
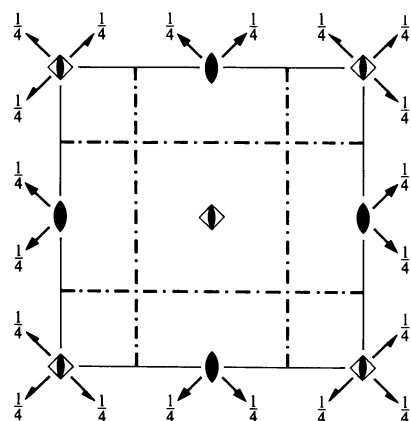
$\bar{4}m2$

Tetragonal

No. 118

$P\bar{4}n2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|--|--|--|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $\bar{4}^+$ $0, 0, z$; $0, 0, 0$ | (4) $\bar{4}^-$ $0, 0, z$; $0, 0, 0$ |
| (5) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (6) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 <i>i</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) y, \bar{x}, \bar{z} (4) \bar{y}, x, \bar{z} (5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	General: $Ok l : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
4 <i>h</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>g</i> ..2	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	no extra conditions
4 <i>f</i> ..2	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$	no extra conditions
4 <i>e</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
2 <i>d</i> 2..22	$0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$	$hkl : h + k + l = 2n$
2 <i>c</i> 2..22	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>b</i> $\bar{4}$..	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[110]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2n1$ ($Pnn2$, 34) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIIb [2] $F\bar{4}d2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}2d$, 122)

Maximal isomorphic subgroups of lowest index

IIIc [3] $P\bar{4}n2$ ($\mathbf{c}' = 3\mathbf{c}$) (118); [9] $P\bar{4}n2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (118)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4/mnc$ (128); [2] $P4_2/nnm$ (134); [2] $P4_2/mnm$ (136)

II [2] $C\bar{4}c2$ ($P\bar{4}2c$, 112); [2] $I\bar{4}m2$ (119); [2] $P\bar{4}b2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (117)

$I\bar{4}m2$

D_{2d}^9

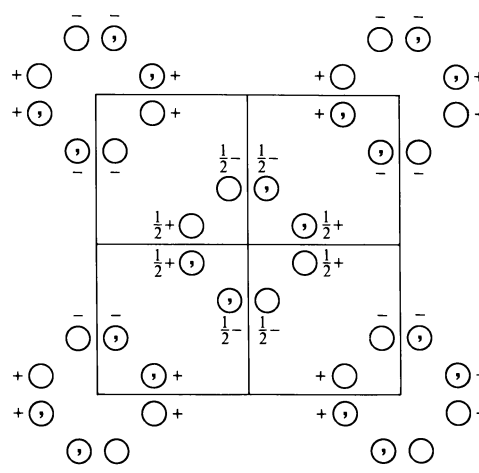
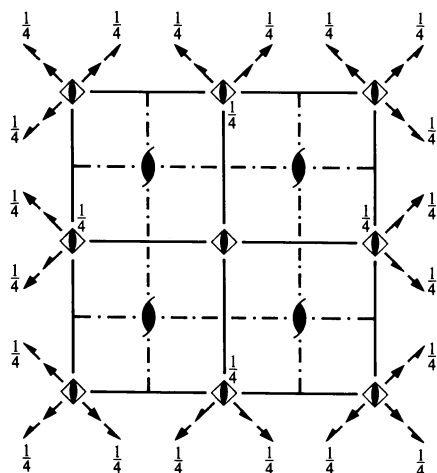
$\bar{4}m2$

Tetragonal

No. 119

$I\bar{4}m2$

Patterson symmetry $I4/mmm$



Origin at $\bar{4}m2$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|----------------|----------------|------------------------------|------------------------------|
| (1) 1 | (2) $2\ 0,0,z$ | (3) $\bar{4}^+ 0,0,z; 0,0,0$ | (4) $\bar{4}^- 0,0,z; 0,0,0$ |
| (5) $m\ x,0,z$ | (6) $m\ 0,y,z$ | (7) $2\ x,x,0$ | (8) $2\ x,\bar{x},0$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- | | | | |
|---|---|--|--|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})\ \frac{1}{4},\frac{1}{4},z$ | (3) $\bar{4}^+ \frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$ | (4) $\bar{4}^- 0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$ |
| (5) $n(\frac{1}{2},0,\frac{1}{2})\ x,\frac{1}{4},z$ | (6) $n(0,\frac{1}{2},\frac{1}{2})\ \frac{1}{4},y,z$ | (7) $2(\frac{1}{2},\frac{1}{2},0)\ x,x,\frac{1}{4}$ | (8) $2\ x,\bar{x}+\frac{1}{2},\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16	<i>j</i> 1	(1) x, y, z (5) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z	(3) y, \bar{x}, \bar{z} (7) y, x, \bar{z}	(4) \bar{y}, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8	<i>i</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, \bar{x}, \bar{z}$	$0, x, \bar{z}$	Special: no extra conditions
8	<i>h</i> . . 2	$x, x + \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	
8	<i>g</i> . . 2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$x, \bar{x}, 0$	$\bar{x}, x, 0$	
4	<i>f</i> 2 <i>m m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			
4	<i>e</i> 2 <i>m m</i> .	$0, 0, z$	$0, 0, \bar{z}$			
2	<i>d</i> $\bar{4}m2$	$0, \frac{1}{2}, \frac{3}{4}$				
2	<i>c</i> $\bar{4}m2$	$0, \frac{1}{2}, \frac{1}{4}$				
2	<i>b</i> $\bar{4}m2$	$0, 0, \frac{1}{2}$				
2	<i>a</i> $\bar{4}m2$	$0, 0, 0$				

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $c1m1$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}11$ ($I\bar{4}$, 82)	(1; 2; 3; 4)+
	[2] $I2m1$ ($Imm2$, 44)	(1; 2; 5; 6)+
	[2] $I212$ ($F222$, 22)	(1; 2; 7; 8)+
IIa	[2] $P\bar{4}n2$ (118)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P\bar{4}m2$ (115)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P\bar{4}m2$ (115)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}m2$ ($\mathbf{c}' = 3\mathbf{c}$) (119); [9] $I\bar{4}m2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (119)

Minimal non-isomorphic supergroups

I	[2] $I4/mmm$ (139); [2] $I4_1/amd$ (141); [3] $F\bar{4}3m$ (216)
II	[2] $C\bar{4}m2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P\bar{4}2m$, 111)

$I\bar{4}c2$

D_{2d}^{10}

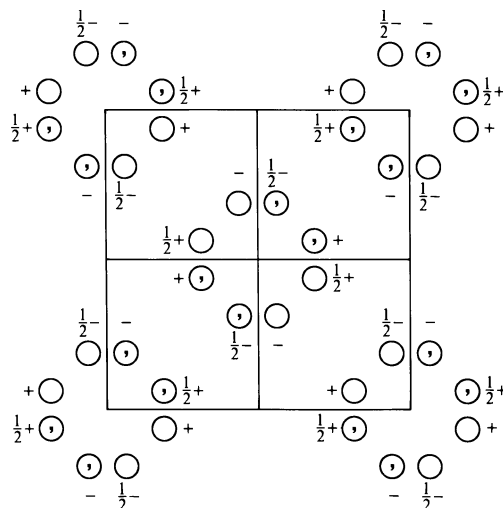
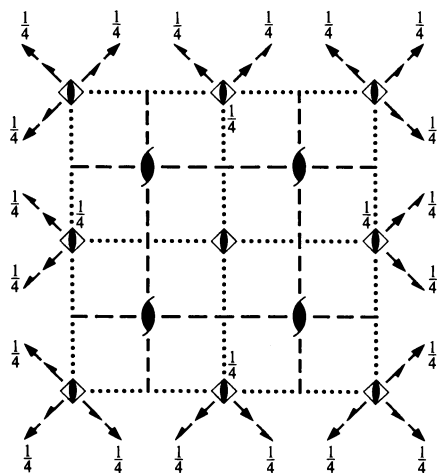
$\bar{4}m2$

Tetragonal

No. 120

$I\bar{4}c2$

Patterson symmetry $I4/mmm$



Origin at $\bar{4}c2_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---------------|---------------|--------------------------------|--------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $\bar{4}^+$ $0,0,z; 0,0,0$ | (4) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (5) c $x,0,z$ | (6) c $0,y,z$ | (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- | | | | |
|--|---|--|--|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) 2 $(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ | (3) $\bar{4}^+$ $\frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$ | (4) $\bar{4}^-$ $0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$ |
| (5) a $x,\frac{1}{4},z$ | (6) b $\frac{1}{4},y,z$ | (7) 2 $(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$ | (8) 2 $x,\bar{x}+\frac{1}{2},0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$	General:
16 <i>i</i> 1	(1) x,y,z (2) \bar{x},\bar{y},z (3) y,\bar{x},\bar{z} (4) \bar{y},x,\bar{z} (5) $x,\bar{y},z+\frac{1}{2}$ (6) $\bar{x},y,z+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k,l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$
8 <i>h</i> .. 2	$x,x+\frac{1}{2},0$ $\bar{x},\bar{x}+\frac{1}{2},0$ $x+\frac{1}{2},\bar{x},0$ $\bar{x}+\frac{1}{2},x,0$	Special: as above, plus no extra conditions
8 <i>g</i> 2..	$0,\frac{1}{2},z$ $\frac{1}{2},0,\bar{z}$ $0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$hkl : l=2n$
8 <i>f</i> 2..	$0,0,z$ $0,0,\bar{z}$ $0,0,z+\frac{1}{2}$ $0,0,\bar{z}+\frac{1}{2}$	$hkl : l=2n$
8 <i>e</i> .. 2	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{1}{4}$ $x,\bar{x},\frac{3}{4}$ $\bar{x},x,\frac{3}{4}$	no extra conditions
4 <i>d</i> 2.22	$0,\frac{1}{2},0$ $\frac{1}{2},0,0$	$hkl : l=2n$
4 <i>c</i> $\bar{4}$..	$0,\frac{1}{2},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$	$hkl : l=2n$
4 <i>b</i> $\bar{4}$..	$0,0,0$ $0,0,\frac{1}{2}$	$hkl : l=2n$
4 <i>a</i> 2.22	$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	$hkl : l=2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0,0,z$

Along [100] $p1m1$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x,0,0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}11$ ($I\bar{4}$, 82)	(1; 2; 3; 4)+
	[2] $I2c1$ ($Iba2$, 45)	(1; 2; 5; 6)+
	[2] $I212$ ($F222$, 22)	(1; 2; 7; 8)+
IIa	[2] $P\bar{4}b2$ (117)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}c2$ (116)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P\bar{4}c2$ (116)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}c2$ ($\mathbf{c}' = 3\mathbf{c}$) (120); [9] $I\bar{4}c2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (120)

Minimal non-isomorphic supergroups

I [2] $I4/mcm$ (140); [2] $I4_1/acd$ (142); [3] $F\bar{4}3c$ (219)

II [2] $C\bar{4}m2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P\bar{4}2m$, 111)

$I\bar{4}2m$

D_{2d}^{11}

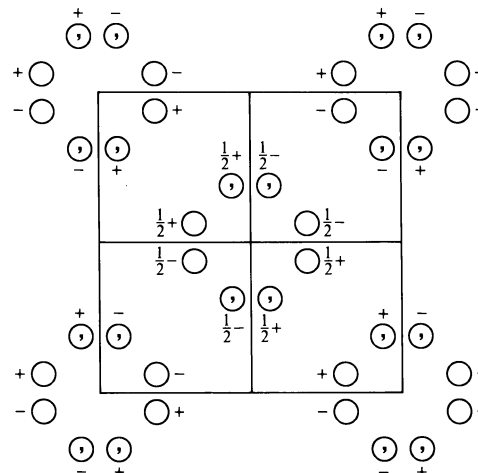
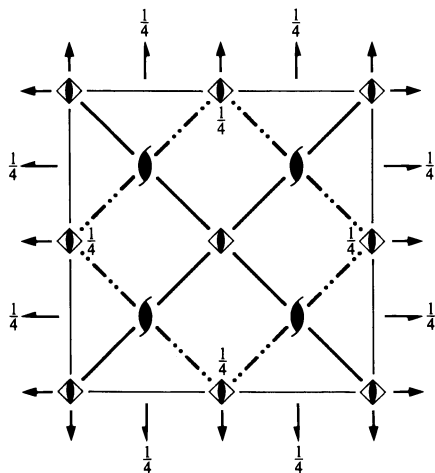
$\bar{4}2m$

Tetragonal

No. 121

$I\bar{4}2m$

Patterson symmetry $I4/mmm$



Origin at $\bar{4}2m$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; x \leq y$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---------------|---------------|--------------------------------|--------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) $\bar{4}^+$ $0,0,z; 0,0,0$ | (4) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) m x,\bar{x},z | (8) m x,x,z |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (4) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) c $x + \frac{1}{2}, \bar{x}, z$ | (8) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	<i>j</i> 1	(1) x,y,z (5) \bar{x},y,\bar{z}	(2) \bar{x},\bar{y},z (6) x,\bar{y},\bar{z}	(3) y,\bar{x},\bar{z} (7) \bar{y},\bar{x},z	(4) \bar{y},x,\bar{z} (8) y,x,z	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$
8	<i>i</i> . . <i>m</i>	x,x,z	\bar{x},\bar{x},z	x,\bar{x},\bar{z}	\bar{x},x,\bar{z}	Special: as above, plus no extra conditions
8	<i>h</i> 2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	$hkl : l=2n$
8	<i>g</i> . 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	no extra conditions
8	<i>f</i> . 2 .	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
4	<i>e</i> 2 . <i>mm</i>	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	<i>d</i> $\bar{4}$. .	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			$hkl : l=2n$
4	<i>c</i> 2 2 2 .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			$hkl : l=2n$
2	<i>b</i> $\bar{4}2m$	$0,0,\frac{1}{2}$				no extra conditions
2	<i>a</i> $\bar{4}2m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0,0,z$

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x,0,0$

Along [110] $p1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}11$ ($I\bar{4}$, 82)	(1; 2; 3; 4)+
	[2] $I21m$ ($Fmm2$, 42)	(1; 2; 7; 8)+
	[2] $I221$ ($I222$, 23)	(1; 2; 5; 6)+
IIa	[2] $P\bar{4}2_1c$ (114)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}2_1m$ (113)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}2m$ (111)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}2m$ ($\mathbf{c}' = 3\mathbf{c}$) (121); [9] $I\bar{4}2m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (121)

Minimal non-isomorphic supergroups

I	[2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $I\bar{4}3m$ (217)
II	[2] $C\bar{4}2m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P\bar{4}m2$, 115)

$I\bar{4}2d$

D_{2d}^{12}

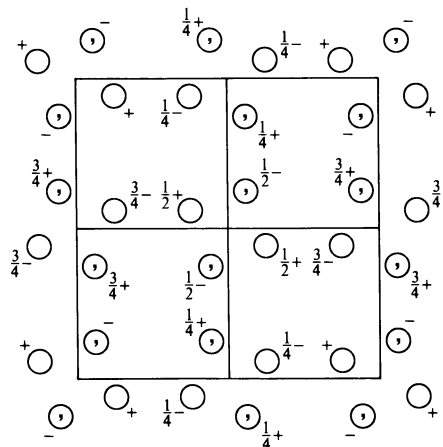
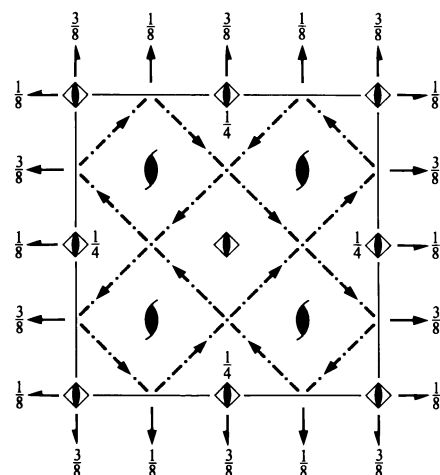
$\bar{4}2m$

Tetragonal

No. 122

$I\bar{4}2d$

Patterson symmetry $I4/mmm$



Origin at $\bar{4}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-------------------------------------|--|---|--|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $\bar{4}^+ \ 0,0,z; \ 0,0,0$ | (4) $\bar{4}^- \ 0,0,z; \ 0,0,0$ |
| (5) $2 \ \frac{1}{4},y,\frac{3}{8}$ | (6) $2(\frac{1}{2},0,0) \ x,0,\frac{3}{8}$ | (7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4}) \ x+\frac{1}{4},\bar{x},z$ | (8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4}) \ x+\frac{1}{4},x,z$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- | | | | |
|--|--|---|--|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2}) \ \frac{1}{4},\frac{1}{4},z$ | (3) $\bar{4}^+ \ \frac{1}{2},0,z; \ \frac{1}{2},0,\frac{1}{4}$ | (4) $\bar{4}^- \ 0,\frac{1}{2},z; \ 0,\frac{1}{2},\frac{1}{4}$ |
| (5) $2(0,\frac{1}{2},0) \ 0,y,\frac{1}{8}$ | (6) $2 \ x,\frac{1}{4},\frac{1}{8}$ | (7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4}) \ x+\frac{1}{4},\bar{x},z$ | (8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4}) \ x-\frac{1}{4},x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16 <i>e</i> 1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(2) \bar{x},\bar{y},z (6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{3}{4}$	(3) y,\bar{x},\bar{z} (7) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(4) \bar{y},x,\bar{z} (8) $y+\frac{1}{2},x,z+\frac{3}{4}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : 2h+l=4n$ $00l : l=4n$ $h00 : h=2n$ $h\bar{h}0 : h=2n$
8 <i>d</i> .2.	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x},\frac{3}{4},\frac{1}{8}$	$\frac{1}{4},\bar{x},\frac{7}{8}$	$\frac{3}{4},x,\frac{7}{8}$	Special: as above, plus no extra conditions
8 <i>c</i> 2..	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},0,z+\frac{3}{4}$	$hkl : l=2n+1$ or $2h+l=4n$
4 <i>b</i> $\bar{4}$..	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$			$hkl : l=2n+1$ or $2h+l=4n$
4 <i>a</i> $\bar{4}$..	$0,0,0$	$\frac{1}{2},0,\frac{3}{4}$			$hkl : l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0,0,z$

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x,0,\frac{3}{8}$

Along [110] $c1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x,x,0$

Maximal non-isomorphic subgroups

- I** [2] $I\bar{4}11$ ($I\bar{4}$, 82) (1; 2; 3; 4)+
 [2] $I21d$ ($Fdd2$, 43) (1; 2; 7; 8)+
 [2] $I221$ ($I2_12_12_1$, 24) (1; 2; 5; 6)+

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

- IIc** [3] $I\bar{4}2d$ ($\mathbf{c}' = 3\mathbf{c}$) (122); [9] $I\bar{4}2d$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (122)

Minimal non-isomorphic supergroups

- I** [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $I\bar{4}3d$ (220)
II [2] $C\bar{4}2d$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P\bar{4}n2$, 118)

$P4/mmm$

D_{4h}^1

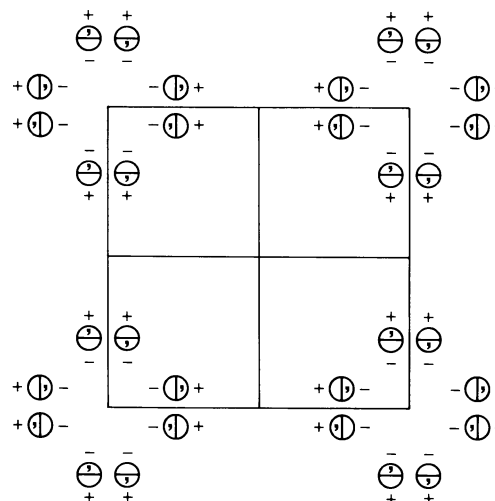
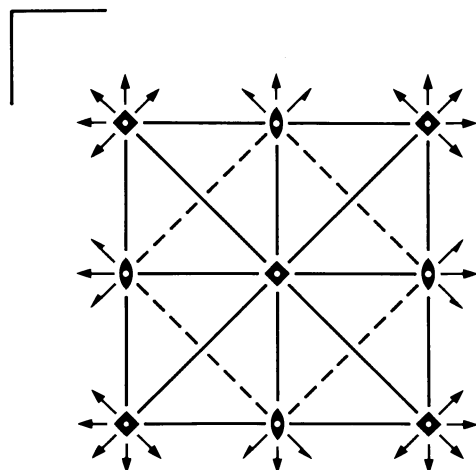
$4/mmm$

Tetragonal

No. 123

$P 4/m 2/m 2/m$

Patterson symmetry $P4/mmm$



Origin at centre ($4/mmm$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; x \leq y$

Symmetry operations

- | | | | |
|--------------|--------------|----------------------------------|----------------------------------|
| (1) 1 | (2) 2 0,0,z | (3) 4 ⁺ 0,0,z | (4) 4 ⁻ 0,0,z |
| (5) 2 0,y,0 | (6) 2 x,0,0 | (7) 2 x,x,0 | (8) 2 x,x̄,0 |
| (9) 1̄ 0,0,0 | (10) m x,y,0 | (11) 4 ⁺ 0,0,z; 0,0,0 | (12) 4 ⁻ 0,0,z; 0,0,0 |
| (13) m x,0,z | (14) m 0,y,z | (15) m x,x̄,z | (16) m x,x,z |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{4}m2$ (115) 1; 2; 7; 8; 11; 12; 13; 14
 [2] $P\bar{4}2m$ (111) 1; 2; 5; 6; 11; 12; 15; 16
 [2] $P4mm$ (99) 1; 2; 3; 4; 13; 14; 15; 16
 [2] $P422$ (89) 1; 2; 3; 4; 5; 6; 7; 8
 [2] $P4/m11$ ($P4/m$, 83) 1; 2; 3; 4; 9; 10; 11; 12
 [2] $P2/m12/m$ ($Cmmm$, 65) 1; 2; 7; 8; 9; 10; 15; 16
 [2] $P2/m2/m1$ ($Pmmm$, 47) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

- IIb** [2] $P4_2/mcm$ ($c' = 2c$) (132); [2] $P4_2/mmc$ ($c' = 2c$) (131); [2] $P4/mcc$ ($c' = 2c$) (124);
 [2] $C4/emm$ ($a' = 2a, b' = 2b$) ($P4/nmm$, 129); [2] $C4/mmd$ ($a' = 2a, b' = 2b$) ($P4/mbm$, 127);
 [2] $C4/emd$ ($a' = 2a, b' = 2b$) ($P4/nbm$, 125); [2] $F4/mmc$ ($a' = 2a, b' = 2b, c' = 2c$) ($I4/mcm$, 140);
 [2] $F4/mmm$ ($a' = 2a, b' = 2b, c' = 2c$) ($I4/mmm$, 139)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $P4/mmm$ ($c' = 2c$) (123); [2] $C4/mmm$ ($a' = 2a, b' = 2b$) ($P4/mmm$, 123)

Minimal non-isomorphic supergroups

- I** [3] $Pm\bar{3}m$ (221)
II [2] $I4/mmm$ (139)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
16	<i>u</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x}, \bar{y}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) x, y, \bar{z} (14) \bar{x}, y, z	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	General: no conditions
8	<i>t</i> . <i>m</i> .	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$	$\bar{x}, \frac{1}{2}, z$ $x, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, x, z$ $\frac{1}{2}, x, \bar{z}$	$\frac{1}{2}, \bar{x}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$	Special: no extra conditions
8	<i>s</i> . <i>m</i> .	$x, 0, z$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z$ $x, 0, \bar{z}$	$0, x, z$ $0, x, \bar{z}$	$0, \bar{x}, z$ $0, \bar{x}, \bar{z}$	no extra conditions
8	<i>r</i> . . <i>m</i>	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	\bar{x}, x, z x, x, \bar{z}	x, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8	<i>q</i> <i>m</i> . .	$x, y, \frac{1}{2}$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	<i>p</i> <i>m</i> . .	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
4	<i>o</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>n</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	<i>m</i> <i>m</i> 2 <i>m</i> .	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>l</i> <i>m</i> 2 <i>m</i> .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	<i>k</i> <i>m</i> . 2 <i>m</i>	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>j</i> <i>m</i> . 2 <i>m</i>	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
4	<i>i</i> 2 <i>m</i> <i>m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : h + k = 2n$
2	<i>h</i> 4 <i>m</i> <i>m</i>	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions
2	<i>g</i> 4 <i>m</i> <i>m</i>	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
2	<i>f</i> <i>m</i> <i>m</i> <i>m</i> .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : h + k = 2n$
2	<i>e</i> <i>m</i> <i>m</i> <i>m</i> .	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k = 2n$
1	<i>d</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				no extra conditions
1	<i>c</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
1	<i>b</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, \frac{1}{2}$				no extra conditions
1	<i>a</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, 0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

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$P4/mcc$

D_{4h}^2

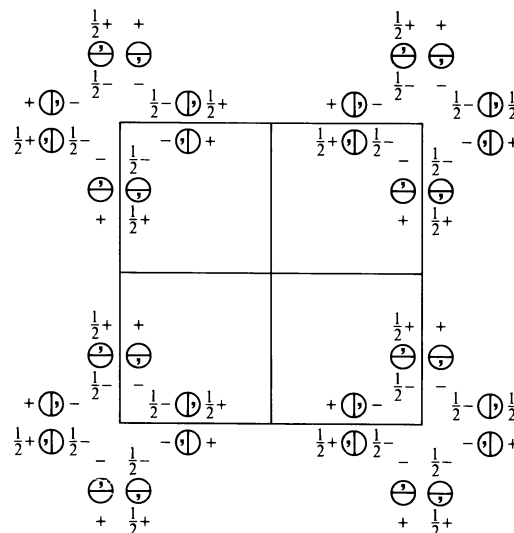
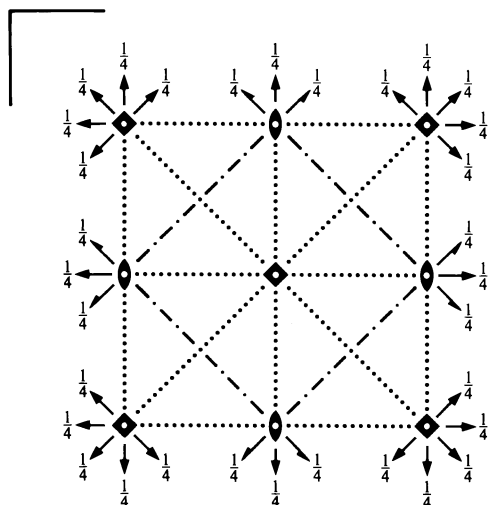
$4/mmm$

Tetragonal

No. 124

$P 4/m 2/c 2/c$

Patterson symmetry $P4/mmm$



Origin at centre ($4/m$) at $4/mcc$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---------------------------|---------------------------|-------------------------------------|-------------------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, 0, z$ | (4) 4^- $0, 0, z$ |
| (5) 2 $0, y, \frac{1}{4}$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}$ $0, 0, 0$ | (10) m $x, y, 0$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) c $x, 0, z$ | (14) c $0, y, z$ | (15) c x, \bar{x}, z | (16) c x, x, z |

Maximal isomorphic subgroups of lowest index

IIc [2] $C4/mcc$ ($a' = 2a, b' = 2b$) ($P4/mcc$, 124); [3] $P4/mcc$ ($c' = 3c$) (124)

Minimal non-isomorphic supergroups

I none

II [2] $I4/mcm$ (140); [2] $P4/mmm$ ($c' = \frac{1}{2}c$) (123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>n</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{y}, x, z (4) y, \bar{x}, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z} (11) y, \bar{x}, \bar{z} (12) \bar{y}, x, \bar{z} (13) $x, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	General: $0kl : l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
8 <i>m</i> $m..$	$x, y, 0$ $\bar{x}, y, \frac{1}{2}$ $y, x, 0$ $\bar{y}, x, \frac{1}{2}$	
8 <i>l</i> $.2.$	$x, \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, x, \frac{1}{4}$ $\frac{1}{2}, \bar{x}, \frac{3}{4}$	$hkl : l = 2n$
8 <i>k</i> $.2.$	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$ $0, x, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$	$hkl : l = 2n$
8 <i>j</i> $..2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$ $\bar{x}, x, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$	$hkl : l = 2n$
8 <i>i</i> $2..$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>h</i> $4..$	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>g</i> $4..$	$0, 0, z$ $0, 0, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>f</i> $222.$	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>e</i> $2/m..$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, l = 2n$
2 <i>d</i> $4/m..$	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n$
2 <i>c</i> 422	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : l = 2n$
2 <i>b</i> $4/m..$	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : l = 2n$
2 <i>a</i> 422	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/m11$ ($P4/m$, 83)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Cccm$, 66)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2/c1$ ($Pccm$, 49)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $C4/ecc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/ncc$, 130); [2] $C4/mcd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/mnc$, 128);
[2] $C4/ecd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/nnc$, 126)

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$P4/nbm$

D_{4h}^3

$4/mmm$

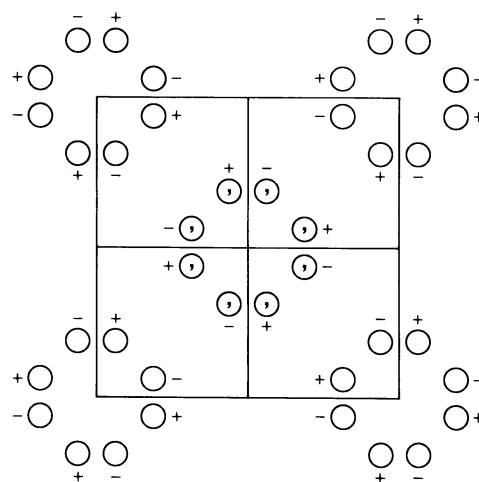
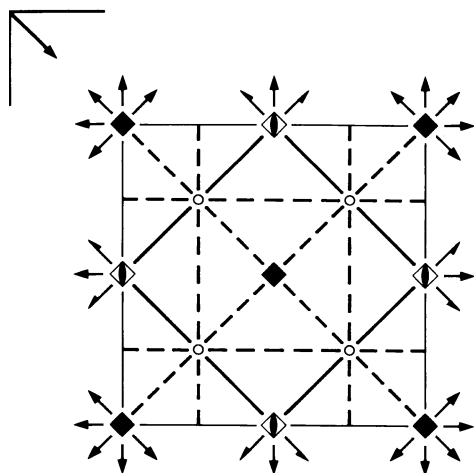
Tetragonal

No. 125

$P 4/n 2/b 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at 422 at $4/n22/g$, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \frac{1}{2} - x$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, 0, z$ | (4) 4^- $0, 0, z$ |
| (5) 2 $0, y, 0$ | (6) 2 $x, 0, 0$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$ | (12) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, 0$ |
| (13) a $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) m $x + \frac{1}{2}, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)$ x, x, z |

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nbm$ ($c' = 2c$) (125); [9] $P4/nbm$ ($a' = 3a, b' = 3b$) (125)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
16 <i>n</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0 : h + k = 2n$ $0kl : k = 2n$ $h00 : h = 2n$
					Special: as above, plus
8 <i>m</i> .. <i>m</i>	$x, x + \frac{1}{2}, z$ $\bar{x}, x + \frac{1}{2}, \bar{z}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x, \bar{x} + \frac{1}{2}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x, \bar{z}$	$x + \frac{1}{2}, \bar{x}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$	no extra conditions
8 <i>l</i> .2.	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, x, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>k</i> .2.	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$0, x, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0, \bar{x}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>j</i> ..2	$x, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>i</i> ..2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$	$\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 <i>h</i> 2. <i>mm</i>	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : h + k = 2n$
4 <i>g</i> 4..	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hkl : h + k = 2n$
4 <i>f</i> ..2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>e</i> ..2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h, k = 2n$
2 <i>d</i> $\bar{4}2m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>c</i> $\bar{4}2m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : h + k = 2n$
2 <i>b</i> 422	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> 422	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $p2mm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/nm$ ($c' = 2c$) (134); [2] $P4_2/nbc$ ($c' = 2c$) (133); [2] $P4/nnc$ ($c' = 2c$) (126)

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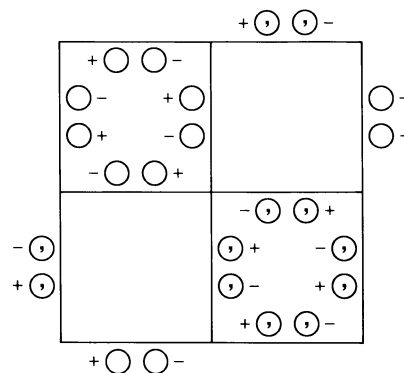
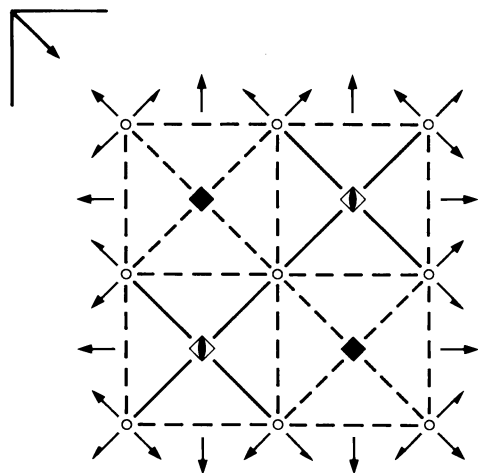
$P4/nbm$ D_{4h}^3 $4/mmm$

Tetragonal

No. 125

 $P 4/n 2/b 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

**Origin** at centre $(2/m)$ at $n(b, a)(2_1/g, 2/m)$, at $\frac{1}{4}, \frac{1}{4}, 0$ from 422**Asymmetric unit** $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq -y$ **Symmetry operations**

- | | | | |
|---------------------------|---|---|---|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 4 ⁺ $\frac{1}{4}, \frac{1}{4}, z$ | (4) 4 ⁻ $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, 0$ | (6) 2 $x, \frac{1}{4}, 0$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1}$ 0, 0, 0 | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ | (12) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$ |
| (13) a $x, 0, z$ | (14) b $0, y, z$ | (15) m x, \bar{x}, z | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)$ x, x, z |

Maximal isomorphic subgroups of lowest index**IIc** [2] $P4/nbm$ ($c' = 2c$) (125); [9] $P4/nbm$ ($a' = 3a, b' = 3b$) (125)**Minimal non-isomorphic supergroups****I** none**II** [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>n</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z$ (4) $y, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (7) y, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$ (14) $\bar{x}, y + \frac{1}{2}, z$ (15) \bar{y}, \bar{x}, z (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0 : h + k = 2n$ $0kl : k = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>m</i> .. <i>m</i>	x, \bar{x}, z $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x, x + \frac{1}{2}, \bar{z}$ $x + \frac{1}{2}, x, z$ \bar{x}, x, \bar{z} $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	no extra conditions
8 <i>l</i> .2.	$x, \frac{1}{4}, \frac{1}{2}$ $\bar{x}, \frac{3}{4}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, x, \frac{1}{2}$ $\frac{3}{4}, \bar{x}, \frac{1}{2}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>k</i> .2.	$x, \frac{1}{4}, 0$ $\bar{x}, \frac{3}{4}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, 0$ $x + \frac{1}{2}, \frac{3}{4}, 0$ $\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{3}{4}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>j</i> ..2	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>i</i> ..2	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, 0$ $x + \frac{1}{2}, \bar{x}, 0$ $x, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 <i>h</i> 2.. <i>mm</i>	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$hkl : h + k = 2n$
4 <i>g</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	$hkl : h + k = 2n$
4 <i>f</i> ..2/ <i>m</i>	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>e</i> ..2/ <i>m</i>	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h, k = 2n$
2 <i>d</i> $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>c</i> $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h + k = 2n$
2 <i>b</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>a</i> 422	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$	$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/nm$ ($\mathbf{c}' = 2\mathbf{c}$) (134); [2] $P4_2/nbc$ ($\mathbf{c}' = 2\mathbf{c}$) (133); [2] $P4/nnc$ ($\mathbf{c}' = 2\mathbf{c}$) (126)

(Continued on preceding page)

$P4/nnc$

D_{4h}^4

$4/mmm$

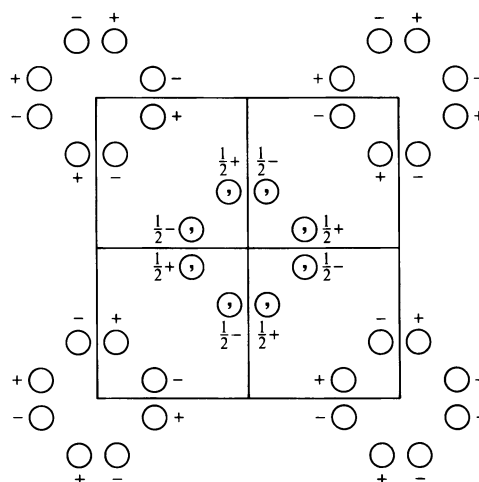
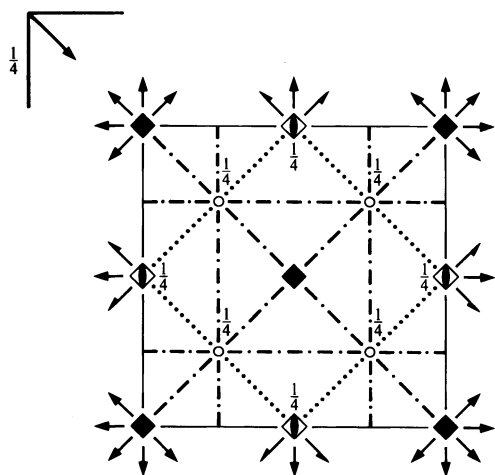
Tetragonal

No. 126

$P 4/n 2/n 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $422/n$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, 0, z$ | (4) 4^- $0, 0, z$ |
| (5) 2 $0, y, 0$ | (6) 2 $x, 0, 0$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (12) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>k</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{y}, x, z (4) y, \bar{x}, z (5) \bar{x}, y, \bar{z} (6) x, \bar{y}, \bar{z} (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>j</i> .2.	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
8 <i>i</i> .2.	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
8 <i>h</i> ..2	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, x, 0$ $x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
8 <i>g</i> 2..	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>f</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h, k, l = 2n$
4 <i>e</i> 4..	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>d</i> $\bar{4}$..	$\frac{1}{2}, 0, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>c</i> 222.	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, l = 2n$
2 <i>b</i> 422	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
2 <i>a</i> 422	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at x, 0, 0

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at x, x, 0

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ($Pnnn$, 48)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/nnc$ ($\mathbf{c}' = 3\mathbf{c}$) (126); [9] $P4/nnc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (126)

Minimal non-isomorphic supergroups

I [3] $Pn\bar{3}n$ (222)

II [2] $I4/mmm$ (139); [2] $C4/mcc$ ($P4/mcc$, 124); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

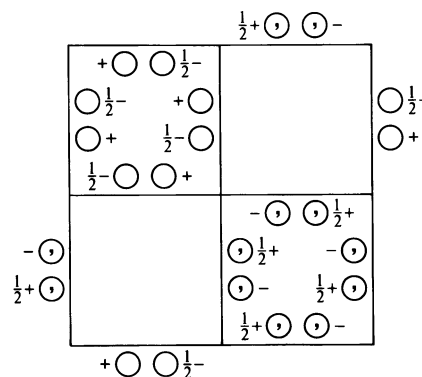
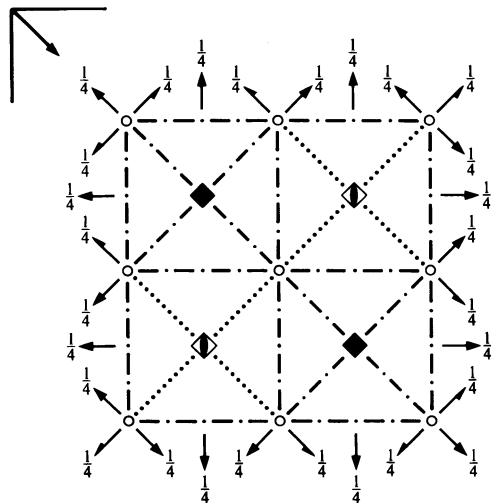
$P4/nnc$ D_{4h}^4 $4/mmm$

Tetragonal

No. 126

 $P 4/n 2/n 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

**Origin** at $\bar{1}$ at $nn(n,c)$, at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from 422**Asymmetric unit** $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$ **Symmetry operations**

- | | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 4^+ $\frac{1}{4}, \frac{1}{4}, z$ | (4) 4^- $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (6) 2 $x, \frac{1}{4}, \frac{1}{4}$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ 0, 0, 0 | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ | (12) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ | (15) c x, \bar{x}, z | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>k</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z$ (4) $y, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	General: $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
8 <i>j</i> .2.	$x, \frac{3}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>i</i> .2.	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>h</i> ..2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>g</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>f</i> $\bar{1}$	0,0,0 $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ 0, $\frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ 0, $\frac{1}{2}, \frac{1}{2}$ 0,0, $\frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k, l = 2n$
4 <i>e</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>d</i> $\bar{4}$..	$\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>c</i> 222.	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
2 <i>b</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ($Pnnn$, 48)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/nnc$ ($\mathbf{c}' = 3\mathbf{c}$) (126); [9] $P4/nnc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (126)

Minimal non-isomorphic supergroups

I [3] $Pn\bar{3}n$ (222)

II [2] $I4/mmm$ (139); [2] $C4/mcc$ ($P4/mcc$, 124); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

$P4/mbm$

D_{4h}^5

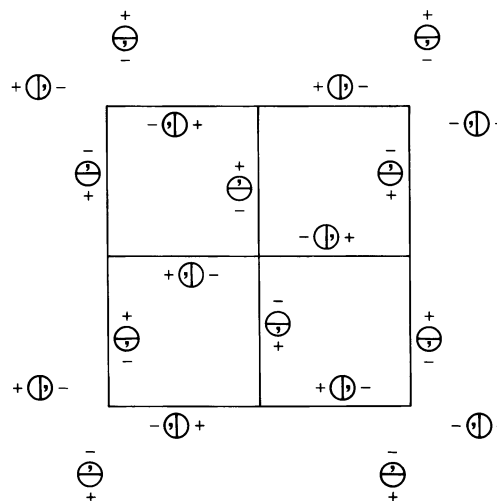
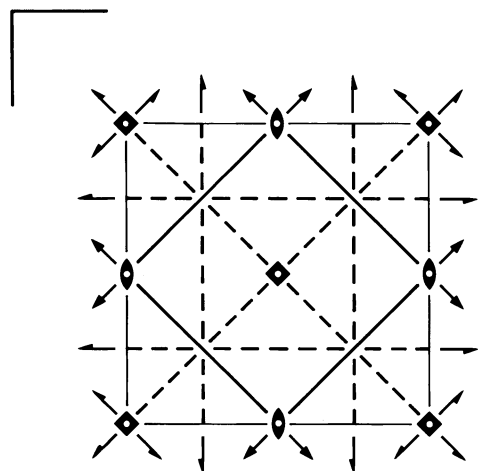
$4/mmm$

Tetragonal

No. 127

$P 4/m 2_1/b 2/m$

Patterson symmetry $P4/mmm$



Origin at centre ($4/m$) at $4/m 12_1/g$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \frac{1}{2} - x$

Symmetry operations

- | | | | |
|--|--|--|---|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (13) a $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) m $x + \frac{1}{2}, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>l</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{y}, x, z (4) y, \bar{x}, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z} (11) y, \bar{x}, \bar{z} (12) \bar{y}, x, \bar{z} (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $Ok_l : k = 2n$ $h00 : h = 2n$
8 <i>k</i> $\dots m$	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$ $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$ $\bar{x} + \frac{1}{2}, x, z$ $x, x + \frac{1}{2}, \bar{z}$ $x + \frac{1}{2}, \bar{x}, z$ $\bar{x}, \bar{x} + \frac{1}{2}, \bar{z}$	Special: as above, plus no extra conditions
8 <i>j</i> $m \dots$	$x, y, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{y}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$ $\bar{y}, x, \frac{1}{2}$ $y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $y, \bar{x}, \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
8 <i>i</i> $m \dots$	$x, y, 0$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$ $\bar{x}, \bar{y}, 0$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$ $\bar{y}, x, 0$ $y + \frac{1}{2}, x + \frac{1}{2}, 0$ $y, \bar{x}, 0$ $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	no extra conditions
4 <i>h</i> $m \dots 2m$	$x, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>g</i> $m \dots 2m$	$x, x + \frac{1}{2}, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, 0$ $x + \frac{1}{2}, \bar{x}, 0$	no extra conditions
4 <i>f</i> $2 \dots mm$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z}$	$hkl : h + k = 2n$
4 <i>e</i> $4 \dots$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$	$hkl : h + k = 2n$
2 <i>d</i> $m \dots mm$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : h + k = 2n$
2 <i>c</i> $m \dots mm$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>b</i> $4/m \dots$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>a</i> $4/m \dots$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at x, 0, 0

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at x, x, 0

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/m11$ ($P4/m$, 83)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/m$ ($Cmmm$, 65)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/b1$ ($Pbam$, 55)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/mnm$ ($\mathbf{c}' = 2\mathbf{c}$) (136); [2] $P4_2/mbc$ ($\mathbf{c}' = 2\mathbf{c}$) (135); [2] $P4/mnc$ ($\mathbf{c}' = 2\mathbf{c}$) (128)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/mbm$ ($\mathbf{c}' = 2\mathbf{c}$) (127); [9] $P4/mbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (127)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

$P4/mnc$

D_{4h}^6

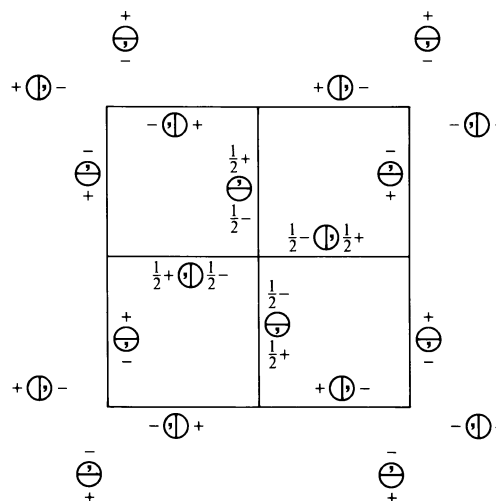
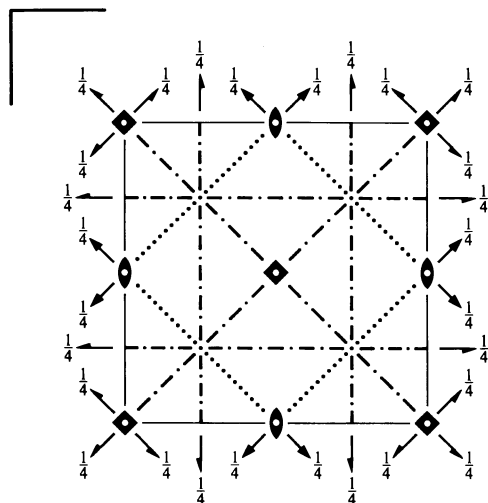
$4/mmm$

Tetragonal

No. 128

$P 4/m 2_1/n 2/c$

Patterson symmetry $P4/mmm$



Origin at centre ($4/m$) at $4/m1n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---|---|--|---|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $4^+ \ 0,0,z$ | (4) $4^- \ 0,0,z$ |
| (5) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \ x, x, \frac{1}{4}$ | (8) $2 \ x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1} \ 0,0,0$ | (10) $m \ x,y,0$ | (11) $4^+ \ 0,0,z; \ 0,0,0$ | (12) $4^- \ 0,0,z; \ 0,0,0$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2}) \ x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2}) \ \frac{1}{4}, y, z$ | (15) $c \ x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
16 <i>i</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) x, y, \bar{z} (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	(3) \bar{y}, x, z (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(4) y, \bar{x}, z (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus
8 <i>h</i> $m..$	$x, y, 0$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\bar{y}, x, 0$ $y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$y, \bar{x}, 0$ $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
8 <i>g</i> $..2$	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$hkl : l = 2n$
8 <i>f</i> $2..$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>e</i> $4..$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>c</i> $2/m..$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$
2 <i>b</i> $4/m..$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2 <i>a</i> $4/m..$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/m11$ ($P4/m$, 83)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Cccm$, 66)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/n1$ ($Pnnm$, 58)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/mnc$ ($\mathbf{c}' = 3\mathbf{c}$) (128); [9] $P4/mnc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (128)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mmm$ (139); [2] $P4/mbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (127)

$P4/nmm$

D_{4h}^7

$4/mmm$

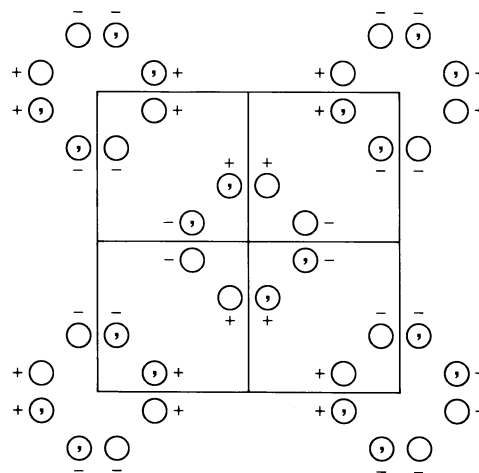
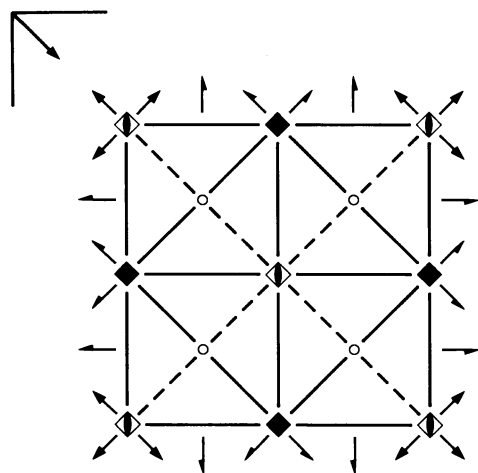
Tetragonal

No. 129

$P 4/n 2_1/m 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}m2$ at $\bar{4}/nm2/g$, at $-\frac{1}{4}, \frac{1}{4}, 0$ from centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \frac{1}{2} - x$

Symmetry operations

- | | | | |
|--|---|--|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, \frac{1}{2}, z$ | (4) 4^- $-\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) m $x, 0, z$ | (14) m $0, y, z$ | (15) m $x + \frac{1}{2}, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 k 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) y, \bar{x}, \bar{z} (12) \bar{y}, x, \bar{z} (13) x, \bar{y}, z (14) \bar{x}, y, z (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	$hk0 : h + k = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 j $..m$	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$ $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$ $\bar{x}, x + \frac{1}{2}, z$ $x + \frac{1}{2}, x, \bar{z}$ $x, \bar{x} + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$	no extra conditions
8 i $.m.$	$0, y, z$ $\frac{1}{2}, y + \frac{1}{2}, \bar{z}$ $0, \bar{y}, z$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, z$ $y, 0, \bar{z}$ $y + \frac{1}{2}, \frac{1}{2}, z$ $\bar{y}, 0, \bar{z}$	no extra conditions
8 h $..2$	$x, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$	$hkl : h + k = 2n$
8 g $..2$	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x, \bar{x}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x, 0$	$hkl : h + k = 2n$
4 f $2mm.$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$	$hkl : h + k = 2n$
4 e $..2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 d $..2/m$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h, k = 2n$
2 c $4mm$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$	no extra conditions
2 b $\bar{4}m2$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
2 a $\bar{4}m2$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ ($Pmnm$, 59)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/n2m$ ($\mathbf{c}' = 2\mathbf{c}$) (138); [2] $P4_2/nmc$ ($\mathbf{c}' = 2\mathbf{c}$) (137); [2] $P4/ncc$ ($\mathbf{c}' = 2\mathbf{c}$) (130)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nmm$ ($\mathbf{c}' = 2\mathbf{c}$) (129); [9] $P4/nmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (129)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mmm$ (139)

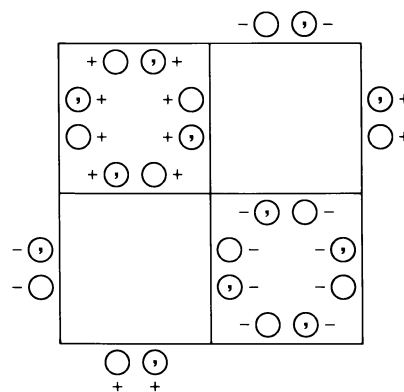
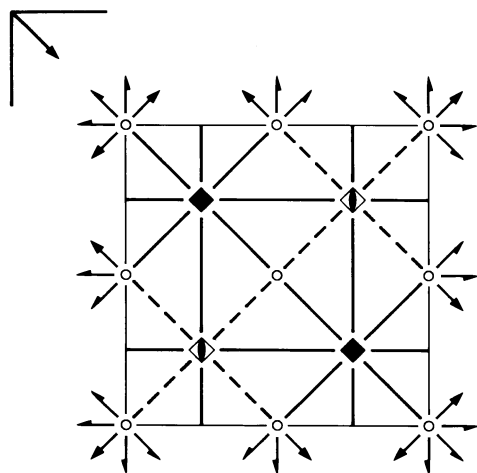
$P4/nmm$ D_{4h}^7 $4/mmm$

Tetragonal

No. 129

 $P 4/n 2_1/m 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2



Origin at centre $(2/m)$ at $n2_1(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}m2$

Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq y$

Symmetry operations

- | | | | |
|------------------------------------|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+ \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^- \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) 0, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (8) $2 x, \bar{x}, 0$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$ |
| (13) $m x, \frac{1}{4}, z$ | (14) $m \frac{1}{4}, y, z$ | (15) $m x + \frac{1}{2}, \bar{x}, z$ | (16) $m x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 k 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z$ (4) $y, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (13) $x, \bar{y} + \frac{1}{2}, z$ (14) $\bar{x} + \frac{1}{2}, y, z$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (16) y, x, z	$hk0 : h + k = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 j $..m$	x, x, z $\bar{x}, x + \frac{1}{2}, \bar{z}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$ $\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $x, \bar{x} + \frac{1}{2}, z$ $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8 i $.m.$	$\frac{1}{4}, y, z$ $\frac{3}{4}, y + \frac{1}{2}, \bar{z}$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, z$ $\frac{3}{4}, \bar{y}, \bar{z}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, z$ $y + \frac{1}{2}, \frac{3}{4}, \bar{z}$ $y, \frac{1}{4}, z$ $\bar{y}, \frac{3}{4}, \bar{z}$	no extra conditions
8 h $..2$	$x, \bar{x}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 g $..2$	$x, \bar{x}, 0$ $\bar{x}, x, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
4 f $2mm.$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$	$hkl : h + k = 2n$
4 e $..2/m$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k = 2n$
4 d $..2/m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h, k = 2n$
2 c $4mm$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	no extra conditions
2 b $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k = 2n$
2 a $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h + k = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along $[100]$ $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ (<i>Cmme</i> , 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ (<i>Pmmn</i> , 59)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/n2m$ ($\mathbf{c}' = 2\mathbf{c}$) (138); [2] $P4_2/nmc$ ($\mathbf{c}' = 2\mathbf{c}$) (137); [2] $P4/ncc$ ($\mathbf{c}' = 2\mathbf{c}$) (130)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nmm$ ($\mathbf{c}' = 2\mathbf{c}$) (129); [9] $P4/nmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (129)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mmm$ (139)

$P4/ncc$

D_{4h}^8

$4/mmm$

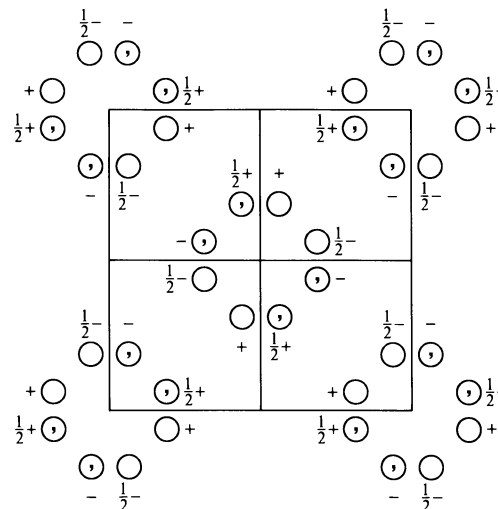
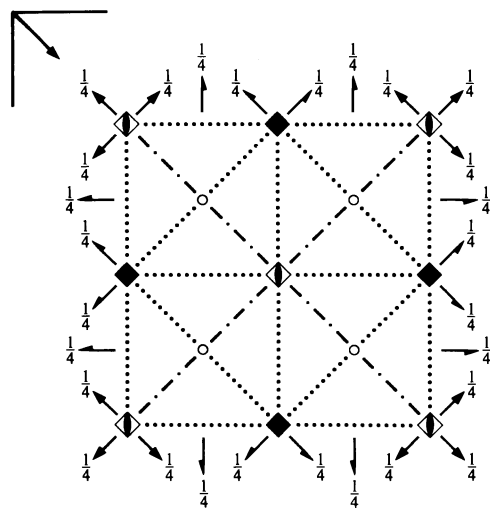
Tetragonal

No. 130

$P 4/n 2_1/c 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}/ncn$, at $-\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|--|--|--------------------------------------|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, \frac{1}{2}, z$ | (4) 4^- $\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) c $x, 0, z$ | (14) c $0, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
16 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (13) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$
	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $0kl : l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$	
			Special: as above, plus
8 <i>f</i> ..2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$ $hkl : h + k + l = 2n$
8 <i>e</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$ $0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $hkl : h + k, l = 2n$
8 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$ $hkl : h, k, l = 2n$
4 <i>c</i> 4..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>b</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>a</i> 2.22	$0, 0, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$ $0, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, \frac{1}{4}, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/ncc$ ($\mathbf{c}' = 3\mathbf{c}$) (130); [9] $P4/ncc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (130)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

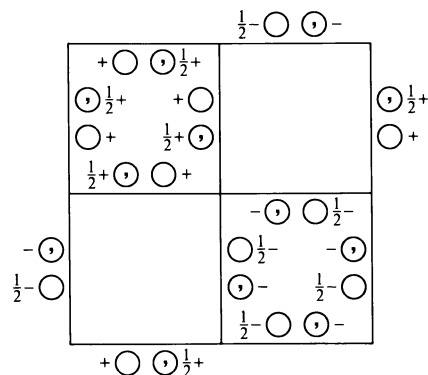
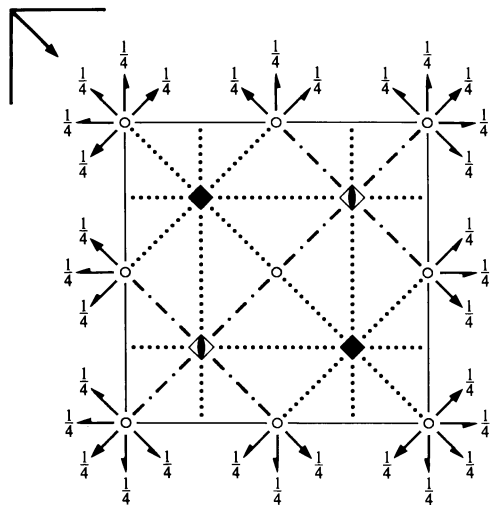
$P4/ncc$ D_{4h}^8 $4/mmm$

Tetragonal

No. 130

 $P 4/n 2_1/c 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $n1(c,n)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|--|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+ \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^- \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, \frac{1}{4}$ | (8) $2 \quad x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1} \quad 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$ |
| (13) $c \quad x, \frac{1}{4}, z$ | (14) $c \quad \frac{1}{4}, y, z$ | (15) $c \quad x + \frac{1}{2}, \bar{x}, z$ | (16) $c \quad x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
16	<i>g</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{y} + \frac{1}{2}, x, z$	(4) $y, \bar{x} + \frac{1}{2}, z$	$hk0 : h + k = 2n$
		(5) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(6) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	$0kl : l = 2n$
		(9) $\bar{x}, \bar{y}, \bar{z}$	(10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(11) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(12) $\bar{y}, x + \frac{1}{2}, \bar{z}$	$hhl : l = 2n$
		(13) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(14) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	(15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(16) $y, x, z + \frac{1}{2}$	$00l : l = 2n$
						$h00 : h = 2n$
						Special: as above, plus
8	<i>f</i> .. 2	$x, \bar{x}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$	$x + \frac{1}{2}, x, \frac{1}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k + l = 2n$
		$\bar{x}, x, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x, x + \frac{1}{2}, \frac{3}{4}$	
8	<i>e</i> 2..	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$hkl : h + k, l = 2n$
		$\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	
8	<i>d</i> $\bar{1}$	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	0, $\frac{1}{2}, 0$	$hkl : h, k, l = 2n$
			$\frac{1}{2}, 0, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	
			$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
4	<i>c</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : l = 2n$
4	<i>b</i> $\bar{4}$..	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4	<i>a</i> 2.22	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/ncc$ ($\mathbf{c}' = 3\mathbf{c}$) (130); [9] $P4/ncc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (130)

Minimal non-isomorphic supergroups

I none

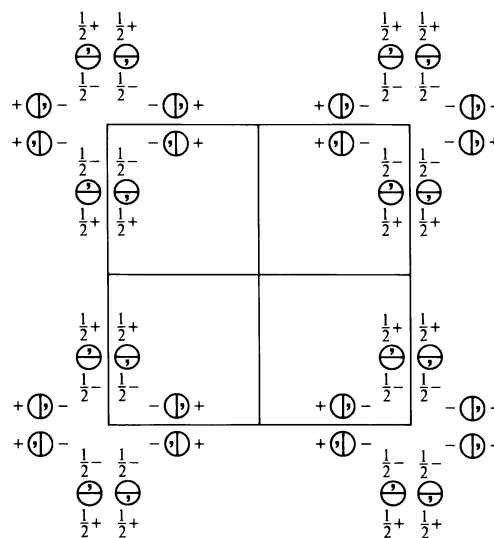
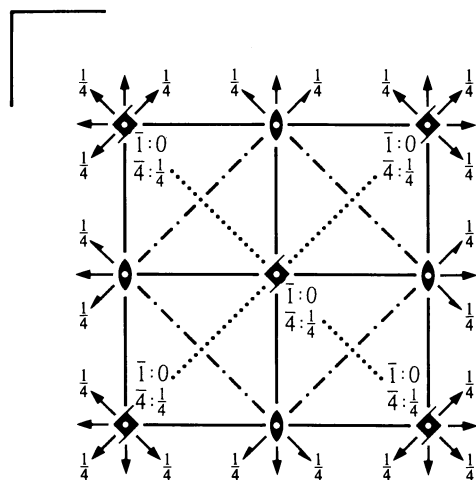
II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

$P4_2/mmc$
 D_{4h}^9
 $4/mmm$

Tetragonal

No. 131

 $P 4_2/m 2/m 2/c$

 Patterson symmetry $P4/mmm$

Origin at centre (mmm) at $4_2/m2/mc$
Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$
Symmetry operations

- | | | | |
|-----------------------|------------------|--|--|
| (1) 1 | (2) 2 $0,0,z$ | (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ | (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |
| (9) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z$; $0,0,\frac{1}{4}$ | (12) $\bar{4}^-$ $0,0,z$; $0,0,\frac{1}{4}$ |
| (13) m $x,0,z$ | (14) m $0,y,z$ | (15) c x,\bar{x},z | (16) c x,x,z |

Maximal non-isomorphic subgroups

- | | | |
|----------|---------------------------------|----------------------------|
| I | [2] $P\bar{4}m2$ (115) | 1; 2; 7; 8; 11; 12; 13; 14 |
| | [2] $P\bar{4}2c$ (112) | 1; 2; 5; 6; 11; 12; 15; 16 |
| | [2] $P4_2mc$ (105) | 1; 2; 3; 4; 13; 14; 15; 16 |
| | [2] $P4_222$ (93) | 1; 2; 3; 4; 5; 6; 7; 8 |
| | [2] $P4_2/m11$ ($P4_2/m$, 84) | 1; 2; 3; 4; 9; 10; 11; 12 |
| | [2] $P2/m12/c$ ($Cccm$, 66) | 1; 2; 7; 8; 9; 10; 15; 16 |
| | [2] $P2/m2/m1$ ($Pmmm$, 47) | 1; 2; 5; 6; 9; 10; 13; 14 |

IIa none

- | | |
|------------|--|
| IIb | [2] $C4_2/emc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nm$, 138); [2] $C4_2/mmd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mnm$, 136); |
| | [2] $C4_2/emd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nm$, 134); [2] $C4_2/mmc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mcm$, 132) |

Maximal isomorphic subgroups of lowest index

- | | |
|------------|---|
| IIc | [3] $P4_2/mmc$ ($\mathbf{c}' = 3\mathbf{c}$) (131); [9] $P4_2/mmc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (131) |
|------------|---|

Minimal non-isomorphic supergroups

- | | |
|-----------|--|
| I | [3] $Pm\bar{3}n$ (223) |
| II | [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (123) |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
16	r 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x}, \bar{y}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) x, y, \bar{z} (14) \bar{x}, y, z	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	$hhl : l = 2n$ $00l : l = 2n$
						Special: as above, plus
8	q $m..$	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	p $.m.$	$\frac{1}{2}, y, z$ $\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, z$ $\frac{1}{2}, \bar{y}, \bar{z}$	$\bar{y}, \frac{1}{2}, z + \frac{1}{2}$ $y, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$y, \frac{1}{2}, z + \frac{1}{2}$ $\bar{y}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8	o $.m.$	$0, y, z$ $0, y, \bar{z}$	$0, \bar{y}, z$ $0, \bar{y}, \bar{z}$	$\bar{y}, 0, z + \frac{1}{2}$ $y, 0, \bar{z} + \frac{1}{2}$	$y, 0, z + \frac{1}{2}$ $\bar{y}, 0, \bar{z} + \frac{1}{2}$	no extra conditions
8	n $..2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x, x, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$ $x, \bar{x}, \frac{1}{4}$	$x, \bar{x}, \frac{3}{4}$ $\bar{x}, x, \frac{1}{4}$	$hkl : l = 2n$
4	m $m2m.$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	l $m2m.$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	k $m2m.$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	j $m2m.$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	i $2mm.$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	h $2mm.$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4	g $2mm.$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
2	f $\bar{4}m2$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2	e $\bar{4}m2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$
2	d $mmm.$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl : h + k + l = 2n$
2	c $mmm.$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	b $mmm.$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	a $mmm.$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at $0, 0, z$

Along $[100]$ $p2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

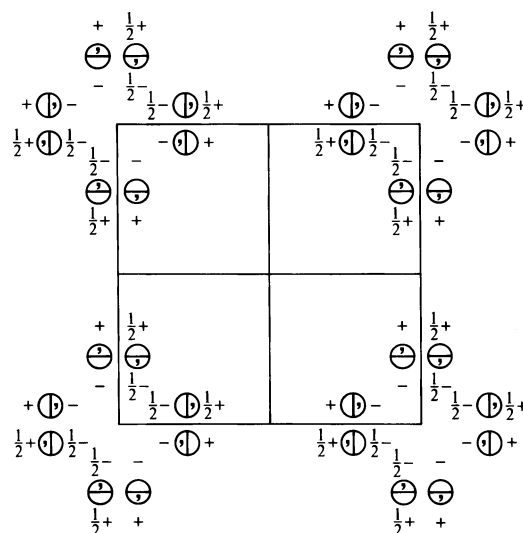
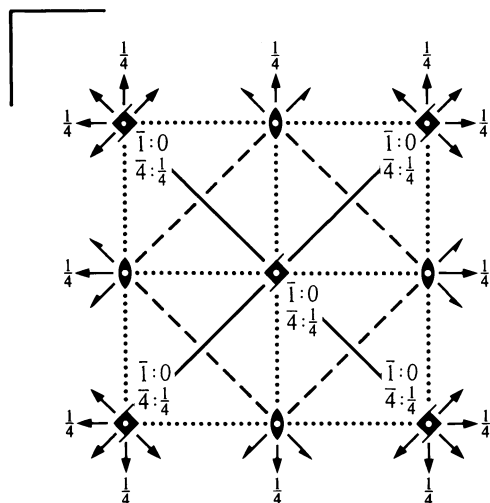
(Continued on preceding page)

$P4_2/mcm$
 D_{4h}^{10}
 $4/mmm$

Tetragonal

No. 132

 $P 4_2/m 2/c 2/m$

 Patterson symmetry $P4/mmm$

Origin at centre (mmm) at $4_2/mc2/m$
Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; x \leq y$
Symmetry operations

- | | | | |
|---------------------------|---------------------------|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, 0, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $0, 0, z$ |
| (5) 2 $0, y, \frac{1}{4}$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |
| (9) $\bar{1}$ $0, 0, 0$ | (10) m $x, y, 0$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, \frac{1}{4}$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, \frac{1}{4}$ |
| (13) c $x, 0, z$ | (14) c $0, y, z$ | (15) m x, \bar{x}, z | (16) m x, x, z |

Maximal non-isomorphic subgroups

- | | | |
|----------|---------------------------------|----------------------------|
| I | [2] $P\bar{4}c2$ (116) | 1; 2; 7; 8; 11; 12; 13; 14 |
| | [2] $P\bar{4}2m$ (111) | 1; 2; 5; 6; 11; 12; 15; 16 |
| | [2] $P4_2cm$ (101) | 1; 2; 3; 4; 13; 14; 15; 16 |
| | [2] $P4_222$ (93) | 1; 2; 3; 4; 5; 6; 7; 8 |
| | [2] $P4_2/m11$ ($P4_2/m$, 84) | 1; 2; 3; 4; 9; 10; 11; 12 |
| | [2] $P2/m12/m$ ($Cmmm$, 65) | 1; 2; 7; 8; 9; 10; 15; 16 |
| | [2] $P2/m2/c1$ ($Pccm$, 49) | 1; 2; 5; 6; 9; 10; 13; 14 |

IIa none

- | | |
|------------|---|
| IIb | [2] $C4_2/ecm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nmc$, 137); [2] $C4_2/mcd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mbc$, 135); |
| | [2] $C4_2/ecd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nbc$, 133); [2] $C4_2/mcm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mmc$, 131) |

Maximal isomorphic subgroups of lowest index

- | | |
|------------|---|
| IIc | [3] $P4_2/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (132); [9] $P4_2/mcm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (132) |
|------------|---|

Minimal non-isomorphic supergroups
I none

- | | |
|-----------|--|
| II | [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mcm$ (140); [2] $P4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (123) |
|-----------|--|

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
16 <i>p</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) x, y, \bar{z} (14) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) y, x, \bar{z} (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ (15) \bar{y}, \bar{x}, z	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$ (16) y, x, z	General: $Ok\bar{l} : l = 2n$ $00l : l = 2n$ Special: as above, plus no extra conditions
8 <i>o</i> $\dots m$	x, x, z $\bar{x}, x, \bar{z} + \frac{1}{2}$	\bar{x}, \bar{x}, z $x, \bar{x}, \bar{z} + \frac{1}{2}$	$\bar{x}, x, z + \frac{1}{2}$ x, x, \bar{z}	$x, \bar{x}, z + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8 <i>n</i> $m \dots$	$x, y, 0$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, \frac{1}{2}$ $y, x, 0$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, 0$	no extra conditions
8 <i>m</i> $\dots 2 \dots$	$x, \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \frac{1}{2}, \frac{1}{4}$ $x, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, x, \frac{3}{4}$ $\frac{1}{2}, \bar{x}, \frac{1}{4}$	$\frac{1}{2}, \bar{x}, \frac{3}{4}$ $\frac{1}{2}, x, \frac{1}{4}$	$hkl : l = 2n$
8 <i>l</i> $\dots 2 \dots$	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x}, 0, \frac{1}{4}$ $x, 0, \frac{3}{4}$	$0, x, \frac{3}{4}$ $0, \bar{x}, \frac{1}{4}$	$0, \bar{x}, \frac{3}{4}$ $0, x, \frac{1}{4}$	$hkl : l = 2n$
8 <i>k</i> $2 \dots$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, z$	$hkl : h + k, l = 2n$
4 <i>j</i> $m \dots 2m$	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
4 <i>i</i> $m \dots 2m$	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>h</i> $2 \dots mm$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$hkl : l = 2n$
4 <i>g</i> $2 \dots mm$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$hkl : l = 2n$
4 <i>f</i> $2/m \dots$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
4 <i>e</i> $222 \dots$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$hkl : h + k, l = 2n$
2 <i>d</i> $\bar{4}2m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2 <i>c</i> $m \dots mm$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2 <i>b</i> $\bar{4}2m$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$
2 <i>a</i> $m \dots mm$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, x, 0$

(Continued on preceding page)

$P4_2/nbc$

D_{4h}^{11}

$4/mmm$

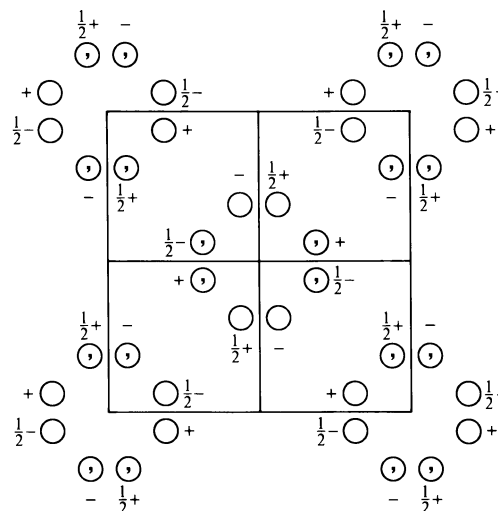
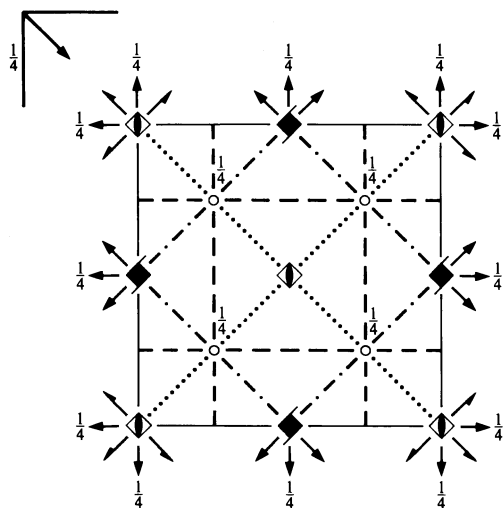
Tetragonal

No. 133

$P 4_2/n 2/b 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}12_1/c$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---|---|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (5) 2 $0, y, \frac{1}{4}$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) a $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) c x, \bar{x}, z | (16) c x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
16 <i>k</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) $y, x, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $0kl : k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus
8 <i>j</i> ..2	$x, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x, \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, 0$	$x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, 0$	$hkl : h + k + l = 2n$
8 <i>i</i> .2.	$x, 0, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$\bar{x}, 0, \frac{3}{4}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $0, \bar{x}, \frac{1}{4}$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $0, x, \frac{1}{4}$	$hkl : h + k = 2n$
8 <i>h</i> .2.	$x, 0, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $0, \bar{x}, \frac{3}{4}$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $0, x, \frac{3}{4}$	$hkl : h + k = 2n$
8 <i>g</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>f</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h, k, l = 2n$
4 <i>d</i> $\bar{4}$..	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, l = 2n$
4 <i>c</i> 2.22	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
4 <i>b</i> 222.	$0, 0, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$0, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>a</i> 222.	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along [100] $p2mm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, \frac{1}{4}$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nbc$ ($\mathbf{c}' = 3\mathbf{c}$) (133); [9] $P4_2/nbc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (133)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

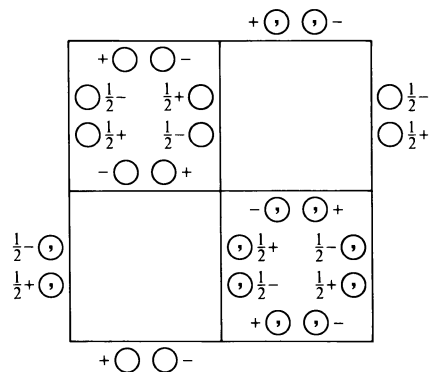
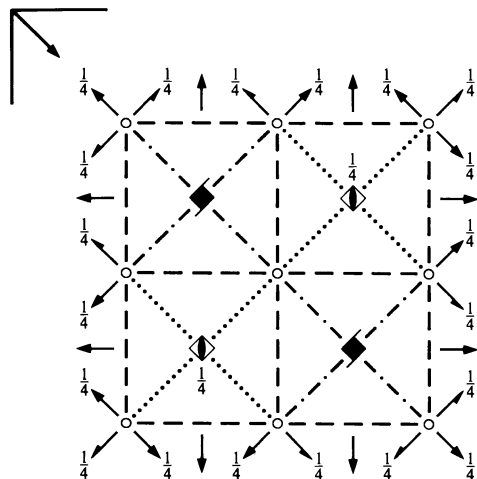
$P4_2/nbc$ D_{4h}^{11} $4/mmm$

Tetragonal

No. 133

 $P 4_2/n 2/b 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $n(b,a)(n,c)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---------------------------|---|---|---|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, 0$ | (6) 2 $x, \frac{1}{4}, 0$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ 0, 0, 0 | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) a $x, 0, z$ | (14) b $0, y, z$ | (15) c x, \bar{x}, z | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions					
		General:									
16	k	1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x}, y + \frac{1}{2}, z$	(3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $Ok1 : k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$				
		Special: as above, plus									
8	j	$\dots 2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k + l = 2n$				
8	i	$. 2 .$	$x, \frac{1}{4}, \frac{1}{2}$ $\bar{x}, \frac{3}{4}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{3}{4}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$				
8	h	$. 2 .$	$x, \frac{1}{4}, 0$ $\bar{x}, \frac{3}{4}, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, 0$ $x + \frac{1}{2}, \frac{3}{4}, 0$	$\frac{1}{4}, x, \frac{1}{2}$ $\frac{3}{4}, \bar{x}, \frac{1}{2}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$				
8	g	$2 \dots$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$				
8	f	$2 \dots$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$				
8	e	$\bar{1}$	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k, l = 2n$	
4	d	$\bar{4} \dots$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$					$hkl : h + k, l = 2n$
4	c	$2 \dots 22$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$					$hkl : h + k, l = 2n$
4	b	$222 \dots$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$					$hkl : h + k, l = 2n$
4	a	$222 \dots$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$					$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIIc [3] $P4_2/nbc$ ($\mathbf{c}' = 3\mathbf{c}$) (133); [9] $P4_2/nbc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (133)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

$P4_2/nnm$
 D_{4h}^{12}
 $4/mmm$

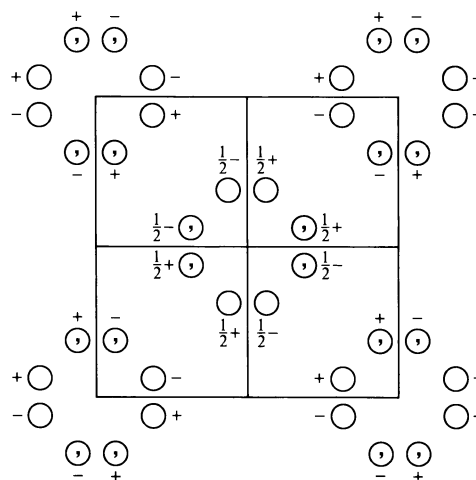
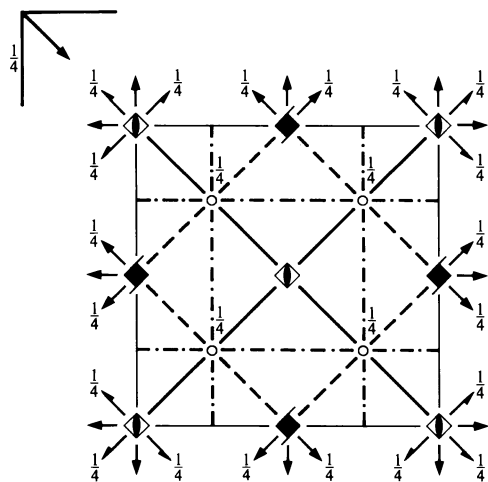
Tetragonal

No. 134

 $P 4_2/n 2/n 2/m$

 Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1


Origin at $\bar{4}2m$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}; x \leq y; y \leq 1-x$
Symmetry operations

- | | | | |
|---|---|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (5) 2 $0, y, 0$ | (6) 2 $x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) $\bar{4}^+ 0, 0, z; 0, 0, 0$ | (12) $\bar{4}^- 0, 0, z; 0, 0, 0$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) m x, \bar{x}, z | (16) m x, x, z |

Maximal non-isomorphic subgroups

- | | | |
|----------|---------------------------------|----------------------------|
| I | [2] $P\bar{4}n2$ (118) | 1; 2; 7; 8; 11; 12; 13; 14 |
| | [2] $P\bar{4}2m$ (111) | 1; 2; 5; 6; 11; 12; 15; 16 |
| | [2] $P4_2nm$ (102) | 1; 2; 3; 4; 13; 14; 15; 16 |
| | [2] $P4_222$ (93) | 1; 2; 3; 4; 5; 6; 7; 8 |
| | [2] $P4_2/n11$ ($P4_2/n$, 86) | 1; 2; 3; 4; 9; 10; 11; 12 |
| | [2] $P2/n12/m$ ($Cmme$, 67) | 1; 2; 7; 8; 9; 10; 15; 16 |
| | [2] $P2/n2/n1$ ($Pnmm$, 48) | 1; 2; 5; 6; 9; 10; 13; 14 |

IIa none

IIb [2] $F4_1/ddc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/acd$, 142); [2] $F4_1/ddm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/amd$, 141)

Maximal isomorphic subgroups of lowest index
IIc [3] $P4_2/nnm$ ($\mathbf{c}' = 3\mathbf{c}$) (134); [9] $P4_2/nnm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (134)

Minimal non-isomorphic supergroups
I [3] $Pn\bar{3}m$ (224)

II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
General:						
16	n 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	$hk0 : h + k = 2n$ $0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
Special: as above, plus						
8	m $\dots m$	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8	l $\dots 2$	$x, x + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$	$\bar{x}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$	$hkl : h + k = 2n$
8	k $\dots 2$	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x, \frac{1}{4}$	$\bar{x}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$hkl : h + k = 2n$
8	j $\dots 2$	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $0, x, \frac{1}{2}$	$hkl : h + k + l = 2n$
8	i $\dots 2$	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $0, \bar{x}, 0$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $0, x, 0$	$hkl : h + k + l = 2n$
8	h $2 \dots$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z$	$hkl : h + k, l = 2n$
4	g $2 \dots mm$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	f $\dots 2/m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4	e $\dots 2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
4	d $2 \dots 22$	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4	c $222 \dots$	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
2	b $\bar{4}2m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2	a $\bar{4}2m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[100]$ $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, \frac{1}{4}$

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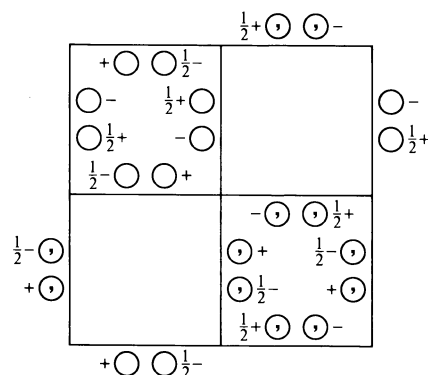
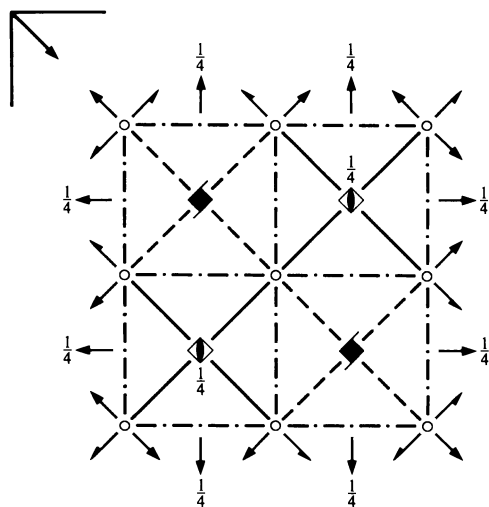
$P4_2/nnm$ D_{4h}^{12} $4/mmm$

Tetragonal

No. 134

 $P 4_2/n 2/n 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

Origin at centre ($2/m$) at $nn(2_1/g, 2/m)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}2m$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq -y$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2 \frac{1}{4}, y, \frac{1}{4}$ | (6) $2 x, \frac{1}{4}, \frac{1}{4}$ | (7) $2 x, x, 0$ | (8) $2 x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2}) x, 0, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ | (15) $m x, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0) x, x, z$ |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{4}n2$ (118) 1; 2; 7; 8; 11; 12; 13; 14
 [2] $P\bar{4}2m$ (111) 1; 2; 5; 6; 11; 12; 15; 16
 [2] $P4_2nm$ (102) 1; 2; 3; 4; 13; 14; 15; 16
 [2] $P4_222$ (93) 1; 2; 3; 4; 5; 6; 7; 8
 [2] $P4_2/n11$ ($P4_2/n$, 86) 1; 2; 3; 4; 9; 10; 11; 12
 [2] $P2/n12/m$ ($Cmme$, 67) 1; 2; 7; 8; 9; 10; 15; 16
 [2] $P2/n2/n1$ ($Pnmm$, 48) 1; 2; 5; 6; 9; 10; 13; 14

IIa none**IIb** [2] $F4_1/ddc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/acd$, 142); [2] $F4_1/ddm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/amd$, 141)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nnm$ ($\mathbf{c}' = 3\mathbf{c}$) (134); [9] $P4_2/nnm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (134)

Minimal non-isomorphic supergroups

- I** [3] $Pn\bar{3}m$ (224)
II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>n</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) y, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) \bar{y}, \bar{x}, z (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8 <i>m</i> $\dots m$	x, \bar{x}, z $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x + \frac{1}{2}, x, z + \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ $x, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ \bar{x}, x, \bar{z} $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	Special: as above, plus no extra conditions
8 <i>l</i> $\dots 2$	$x, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, 0$ $x, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, 0$ $\bar{x}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>k</i> $\dots 2$	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>j</i> $\dots 2.$	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k + l = 2n$
8 <i>i</i> $\dots 2.$	$x, \frac{1}{4}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>h</i> $2 \dots$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z$	$hkl : h + k, l = 2n$
4 <i>g</i> $2 \dots mm$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$hkl : h + k + l = 2n$
4 <i>f</i> $\dots 2/m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>e</i> $\dots 2/m$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>d</i> $2 \dots 22$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>c</i> $222.$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
2 <i>b</i> $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}2m$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along $[100]$ $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

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$P4_2/mbc$

D_{4h}^{13}

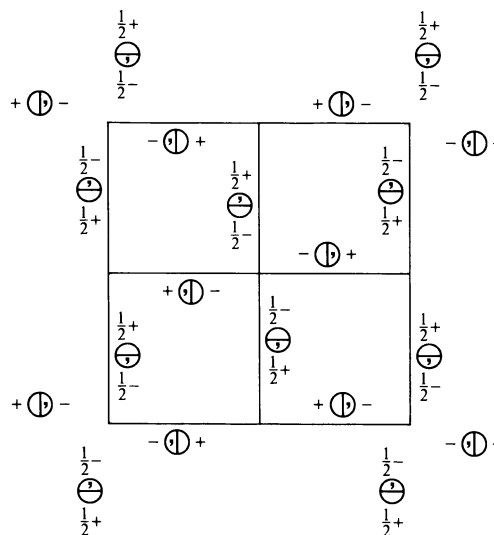
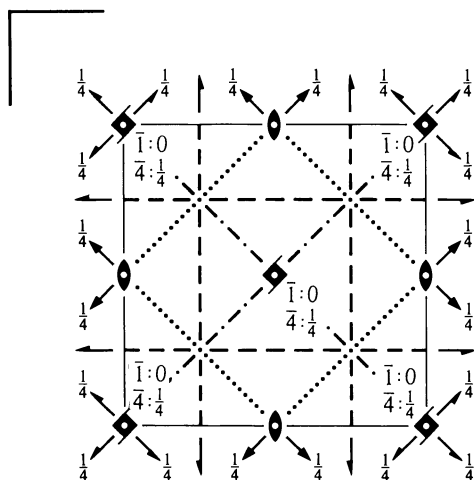
$4/mmm$

Tetragonal

No. 135

$P 4_2/m 2_1/b 2/c$

Patterson symmetry $P4/mmm$



Origin at centre ($2/m$) at $4_2/m 1n$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|--|--|--|---|
| (1) 1 | (2) $2 \ 0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2}) \ 0, 0, z$ | (4) $4^-(0, 0, \frac{1}{2}) \ 0, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \ x, x, \frac{1}{4}$ | (8) $2 \ x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1} \ 0, 0, 0$ | (10) $m \ x, y, 0$ | (11) $4^+ \ 0, 0, z; \ 0, 0, \frac{1}{4}$ | (12) $4^- \ 0, 0, z; \ 0, 0, \frac{1}{4}$ |
| (13) $a \ x, \frac{1}{4}, z$ | (14) $b \ \frac{1}{4}, y, z$ | (15) $c \ x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>i</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y}, x, z + \frac{1}{2}$ (4) $y, \bar{x}, z + \frac{1}{2}$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z} (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	General: $Ok_l : k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8 <i>h</i> $m..$	$x, y, 0$ $\bar{x}, \bar{y}, 0$ $\bar{y}, x, \frac{1}{2}$ $y, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$ $y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	Special: as above, plus no extra conditions
8 <i>g</i> $..2$	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$	$hkl : l = 2n$
8 <i>f</i> $2..$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>e</i> $2..$	$0, 0, z$ $0, 0, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$ $0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$	$hkl : h + k, l = 2n$
4 <i>c</i> $2/m..$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>b</i> $\bar{4}..$	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$hkl : h + k, l = 2n$
4 <i>a</i> $2/m..$	$0, 0, 0$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_1$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 84)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Cccm$, 66)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/b1$ ($Pbam$, 55)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIIc [3] $P4_2/mbc$ ($\mathbf{c}' = 3\mathbf{c}$) (135); [9] $P4_2/mbc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (135)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/mbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (127)

$P4_2/mnm$

D_{4h}^{14}

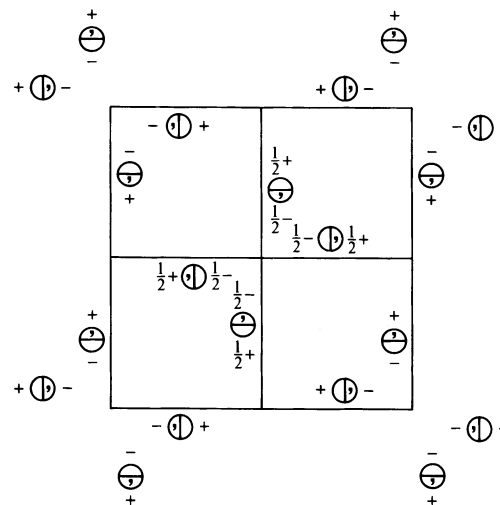
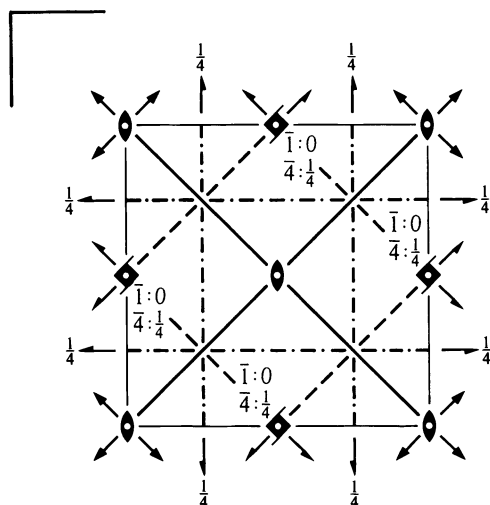
$4/mmm$

Tetragonal

No. 136

$P 4_2/m 2_1/n 2/m$

Patterson symmetry $P4/mmm$



Origin at centre (mmm) at $2/m12/m$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $x \leq y$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $4^+(0,0,\frac{1}{2}) \ 0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{2}) \ \frac{1}{2},0,z$ |
| (5) $2(0,\frac{1}{2},0) \ \frac{1}{4},y,\frac{1}{4}$ | (6) $2(\frac{1}{2},0,0) \ x,\frac{1}{4},\frac{1}{4}$ | (7) $2 \ x,x,0$ | (8) $2 \ x,\bar{x},0$ |
| (9) $\bar{1} \ 0,0,0$ | (10) $m \ x,y,0$ | (11) $\bar{4}^+ \ \frac{1}{2},0,z; \ \frac{1}{2},0,\frac{1}{4}$ | (12) $\bar{4}^- \ 0,\frac{1}{2},z; \ 0,\frac{1}{2},\frac{1}{4}$ |
| (13) $n(\frac{1}{2},0,\frac{1}{2}) \ x,\frac{1}{4},z$ | (14) $n(0,\frac{1}{2},\frac{1}{2}) \ \frac{1}{4},y,z$ | (15) $m \ x,\bar{x},z$ | (16) $m \ x,x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>k</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z} (11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) \bar{y}, \bar{x}, z (16) y, x, z	$0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>j</i> $\dots m$	x, x, z \bar{x}, \bar{x}, z $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ x, x, \bar{z} $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8 <i>i</i> $m \dots$	$x, y, 0$ $\bar{x}, \bar{y}, 0$ $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$ $y, x, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
8 <i>h</i> $2 \dots$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$ $\frac{1}{2}, 0, z$	$hkl : h + k, l = 2n$
4 <i>g</i> $m \cdot 2m$	$x, \bar{x}, 0$ $\bar{x}, x, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>f</i> $m \cdot 2m$	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>e</i> $2 \cdot mm$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$	$hkl : h + k + l = 2n$
4 <i>d</i> $\bar{4} \dots$	$0, \frac{1}{2}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>c</i> $2/m \dots$	$0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
2 <i>b</i> $m \cdot mm$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
2 <i>a</i> $m \cdot mm$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}_2m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_2$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 84)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/m$ ($Cmmm$, 65)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/n1$ ($Pnmm$, 58)	1; 2; 5; 6; 9; 10; 13; 14

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $P4_2/mnm$ ($\mathbf{c}' = 3\mathbf{c}$) (136); [9] $P4_2/mnm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (136)**Minimal non-isomorphic supergroups****I** none**II** [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/mbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (127)

$P4_2/nmc$

D_{4h}^{15}

$4/mmm$

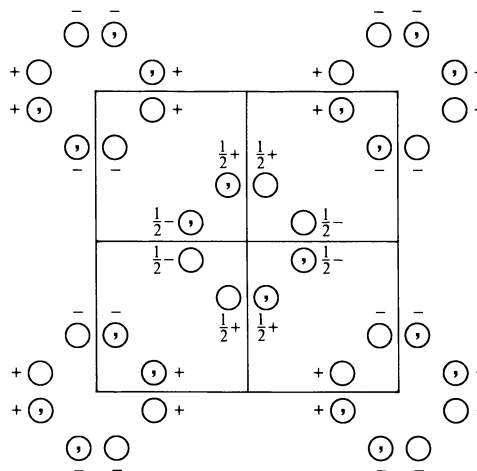
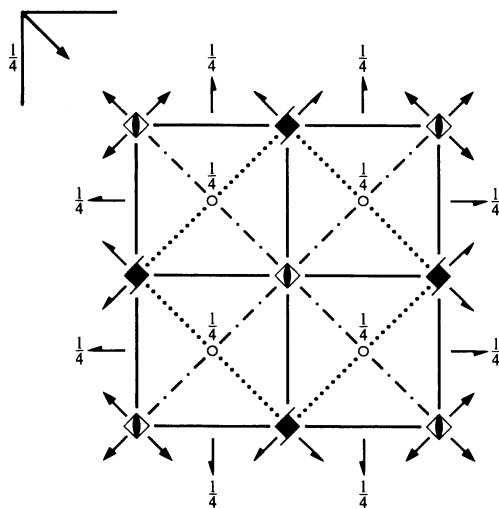
Tetragonal

No. 137

$P 4_2/n 2_1/m 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}m2/n$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|--|---|--|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2}) 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0) \frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) x, \frac{1}{4}, \frac{1}{4}$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |
| (9) $\bar{1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, \frac{1}{4}$ | (11) $\bar{4}^+ 0, 0, z; 0, 0, 0$ | (12) $\bar{4}^- 0, 0, z; 0, 0, 0$ |
| (13) $m x, 0, z$ | (14) $m 0, y, z$ | (15) $c x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>h</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) x, \bar{y}, z	$hk0 : h + k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) \bar{x}, y, z	
	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	
	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	Special: as above, plus
8 <i>g</i> $.m.$	$0, y, z$ $\frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
	$0, \bar{y}, z$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	
	$\bar{y} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $y, 0, \bar{z}$	
	$y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\bar{y}, 0, \bar{z}$	
8 <i>f</i> $. . 2$	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	
	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x, \bar{x}, 0$	
	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x, 0$	
8 <i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h, k, l = 2n$
	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	
	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	
4 <i>d</i> $2mm.$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$	
4 <i>c</i> $2mm.$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$	
2 <i>b</i> $\bar{4}m2$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}m2$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$ Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{4}, \frac{1}{4}$ Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$ **Maximal non-isomorphic subgroups**

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}_2c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ ($Pmnm$, 59)	1; 2; 5; 6; 9; 10; 13; 14

IIa none**IIIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $P4_2/nmc$ ($\mathbf{c}' = 3\mathbf{c}$) (137); [9] $P4_2/nmc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (137)**Minimal non-isomorphic supergroups****I** none**II** [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/nmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

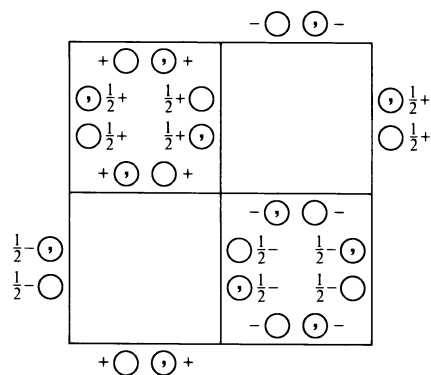
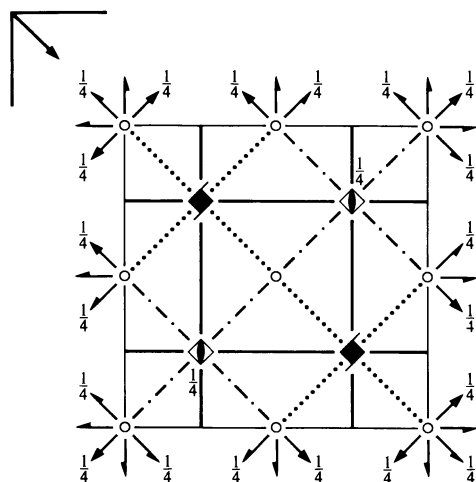
$P4_2/nmc$ D_{4h}^{15} $4/mmm$

Tetragonal

No. 137

 $P 4_2/n 2_1/m 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $n2_1(c,n)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}m2$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|------------------------------------|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) 0, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, \frac{1}{4}$ | (8) $2 x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) $m x, \frac{1}{4}, z$ | (14) $m \frac{1}{4}, y, z$ | (15) $c x + \frac{1}{2}, \bar{x}, z$ | (16) $c x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>h</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y} + \frac{1}{2}, z$ (14) $\bar{x} + \frac{1}{2}, y, z$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	General: $hk0 : h + k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8 <i>g</i> $.m.$	$\frac{1}{4}, y, z$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, z$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}$ $y, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, y + \frac{1}{2}, \bar{z}$ $\frac{3}{4}, \bar{y}, \bar{z}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\bar{y}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	Special: as above, plus no extra conditions
8 <i>f</i> $. . 2$	$x, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k + l = 2n$
8 <i>e</i> $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$hkl : h, k, l = 2n$
4 <i>d</i> $2mm.$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4 <i>c</i> $2mm.$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
2 <i>b</i> $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$ Along [100] $p2mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$ Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$ **Maximal non-isomorphic subgroups**

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ ($Pmnm$, 59)	1; 2; 5; 6; 9; 10; 13; 14

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $P4_2/nmc$ ($\mathbf{c}' = 3\mathbf{c}$) (137); [9] $P4_2/nmc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (137)**Minimal non-isomorphic supergroups****I** none**II** [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/nmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

$P4_2/n\,cm$

D_{4h}^{16}

$4/m\,mm$

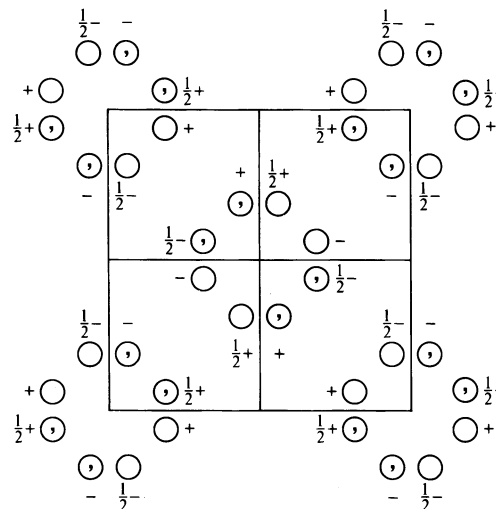
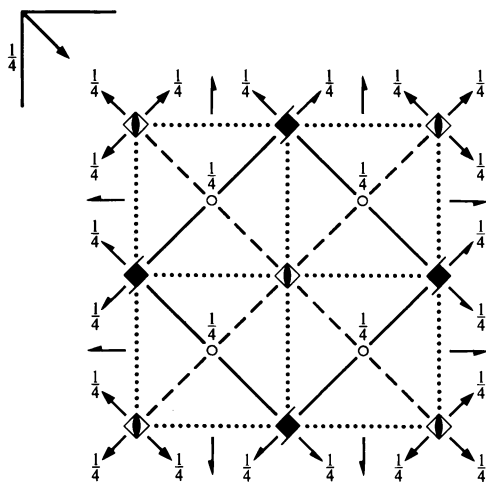
Tetragonal

No. 138

$P\ 4_2/n\ 2_1/c\ 2/m$

Patterson symmetry $P4/m\,mm$

ORIGIN CHOICE 1



Origin at $\bar{4}c$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{4}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $x \leq y$; $y \leq \frac{1}{2} - x$

Symmetry operations

- | | | | |
|--|--|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})\ 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})\ \frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)\ \frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)\ x, \frac{1}{4}, 0$ | (7) $2\ x, x, \frac{1}{4}$ | (8) $2\ x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}\ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)\ x, y, \frac{1}{4}$ | (11) $\bar{4}^+\ 0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-\ 0, 0, z; 0, 0, 0$ |
| (13) $c\ x, 0, z$ | (14) $c\ 0, y, z$ | (15) $m\ x + \frac{1}{2}, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)\ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>j</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $0kl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$	
	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	
	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	
		Special: as above, plus
8 <i>i</i> .. <i>m</i>	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$	no extra conditions
	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$	
	$\bar{x}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	
	$x, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	
8 <i>h</i> .. 2	$x, x, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k = 2n$
	$\bar{x}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	
	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x, \bar{x}, \frac{1}{4}$	
	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x, \frac{1}{4}$	
8 <i>g</i> .. 2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k = 2n$
	$\bar{x}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$	
	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x, \bar{x}, \frac{3}{4}$	
	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	
8 <i>f</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $0, 0, \bar{z}$	
	$\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, z + \frac{1}{2}$	
	$0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z$	
4 <i>e</i> 2.. <i>mm</i>	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
	$\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	
4 <i>d</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	
4 <i>c</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	
4 <i>b</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, 0$ $0, 0, \frac{1}{2}$	
4 <i>a</i> 2.. 22	$0, 0, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $0, 0, \frac{3}{4}$	

Symmetry of special projections

Along [001] $p4\,mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $p2\,mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, \frac{1}{4}, 0$

Along [110] $p2\,mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_2$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n\,cm$ ($\mathbf{c}' = 3\mathbf{c}$) (138); [9] $P4_2/n\,cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (138)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/m\,cm$ ($P4_2/m\,mc$, 131); [2] $I4/m\,cm$ (140); [2] $P4/n\,mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

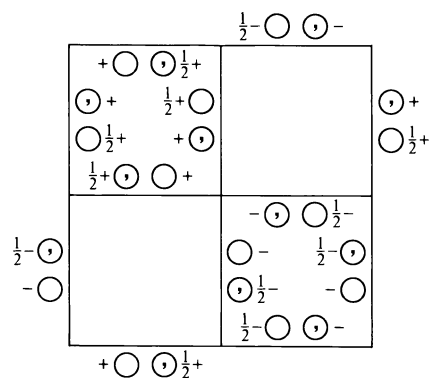
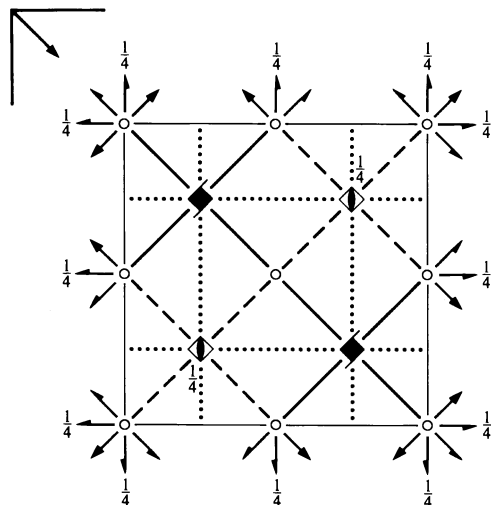
$P4_2/n\bar{c}m$ D_{4h}^{16} $4/m\bar{m}m$

Tetragonal

No. 138

 $P 4_2/n 2_1/c 2/m$ Patterson symmetry $P4/m\bar{m}m$

ORIGIN CHOICE 2



Origin at centre ($2/m$) at $n 1 (2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq y$

Symmetry operations

- | | | | |
|--|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) 0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (8) $2 x, \bar{x}, 0$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) $c x, \frac{1}{4}, z$ | (14) $c \frac{1}{4}, y, z$ | (15) $m x + \frac{1}{2}, \bar{x}, z$ | (16) $m x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>j</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (16) y, x, z	$hk0 : h + k = 2n$ $0kl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>i</i> .. <i>m</i>	x, x, z $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, z + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8 <i>h</i> .. 2	$x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, x, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $x, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>g</i> .. 2	$x, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, 0$ $x, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>f</i> 2..	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, z$	$hkl : h + k, l = 2n$
4 <i>e</i> 2. <i>mm</i>	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	$hkl : l = 2n$
4 <i>d</i> .. 2/ <i>m</i>	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>c</i> .. 2/ <i>m</i>	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>b</i> $\bar{4}$..	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
4 <i>a</i> 2. 22	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4\,mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2\,mg$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, 0, 0$

Along [110] $p2\,mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_2$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n\,cm$ ($\mathbf{c}' = 3\mathbf{c}$) (138); [9] $P4_2/n\,cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (138)

Minimal non-isomorphic supergroups

I none

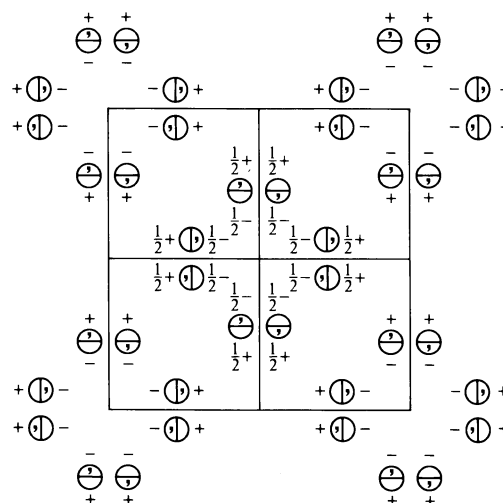
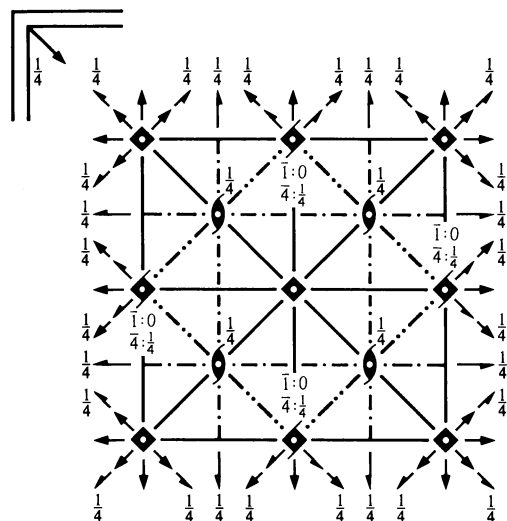
II [2] $C4_2/m\,cm$ ($P4_2/m\,mc$, 131); [2] $I4/m\,cm$ (140); [2] $P4/n\,mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

$I4/mmm$
 D_{4h}^{17}
 $4/mmm$

Tetragonal

No. 139

 $I 4/m 2/m 2/m$

 Patterson symmetry $I4/mmm$

Origin at centre ($4/mmm$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; x \leq y$
Symmetry operations

 For $(0,0,0)+$ set

- | | | | |
|-----------------------|------------------|---------------------------------|---------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,0$ | (8) 2 $x,\bar{x},0$ |
| (9) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (13) m $x,0,z$ | (14) m $0,y,z$ | (15) m x,\bar{x},z | (16) m x,x,z |

 For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|---|---|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0,0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; 0, \frac{1}{2}, \frac{1}{4}$ | (12) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Maximal non-isomorphic subgroups (continued)

- IIa** [2] $P4_2/nmc$ (137) 1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4_2/mnm$ (136) 1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4_2/nnm$ (134) 1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4_2/mmc$ (131) 1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4/nmm$ (129) 1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4/nmc$ (128) 1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4/nnc$ (126) 1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P4/mmm$ (123) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16

IIb none

Maximal isomorphic subgroups of lowest index
IIc [3] $I4/mmm$ ($c' = 3c$) (139); [9] $I4/mmm$ ($a' = 3a, b' = 3b$) (139)

Minimal non-isomorphic supergroups
I [3] $Fm\bar{3}m$ (225); [3] $Im\bar{3}m$ (229)

II [2] $C4/mmm$ ($c' = \frac{1}{2}c$) ($P4/mmm$, 123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates (0,0,0)+ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				Reflection conditions
32 <i>o</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x}, \bar{y}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) x, y, \bar{z} (14) \bar{x}, y, z	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	General: $hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
16 <i>n</i> . <i>m</i> .	$0, y, z$ $0, y, \bar{z}$	$0, \bar{y}, z$ $0, \bar{y}, \bar{z}$	$\bar{y}, 0, z$ $y, 0, \bar{z}$	$y, 0, z$ $\bar{y}, 0, \bar{z}$	no extra conditions
16 <i>m</i> . . <i>m</i>	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	\bar{x}, x, z x, x, \bar{z}	x, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
16 <i>l</i> <i>m</i> . .	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
16 <i>k</i> . . 2	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$hkl : l = 2n$
8 <i>j</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
8 <i>i</i> <i>m</i> 2 <i>m</i> .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
8 <i>h</i> <i>m</i> . 2 <i>m</i>	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
8 <i>g</i> 2 <i>m</i> <i>m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$
8 <i>f</i> . . 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : k, l = 2n$
4 <i>e</i> 4 <i>m</i> <i>m</i>	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
4 <i>d</i> $\bar{4}$ <i>m</i> 2	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$			$hkl : l = 2n$
4 <i>c</i> <i>m</i> <i>m</i> <i>m</i> .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : l = 2n$
2 <i>b</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, \frac{1}{2}$				no extra conditions
2 <i>a</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, 0$				no extra conditions

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at x, 0, 0

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at x, x, 0

Maximal non-isomorphic subgroups

I		
[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+	
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+	
[2] $I4mm$ (107)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+	
[2] $I4/m11$ ($I4/m$, 87)	(1; 2; 3; 4; 9; 10; 11; 12)+	
[2] $I2/m2/m1$ ($Immm$, 71)	(1; 2; 5; 6; 9; 10; 13; 14)+	
[2] $I2/m12/m$ ($Fmmm$, 69)	(1; 2; 7; 8; 9; 10; 15; 16)+	

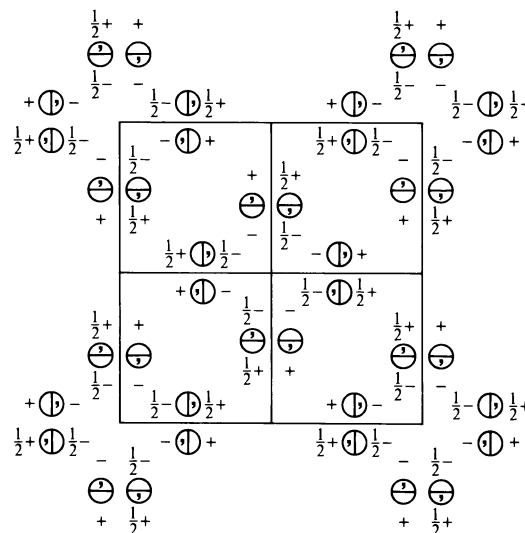
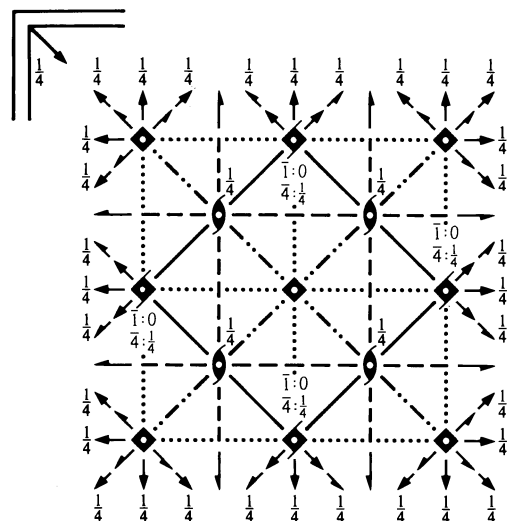
(Continued on preceding page)

$I4/mcm$
 D_{4h}^{18}
 $4/mmm$

Tetragonal

No. 140

 $I 4/m 2/c 2/m$

 Patterson symmetry $I4/mmm$

 Origin at centre ($4/m$) at $4/mc2_1/e$

 Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$; $y \leq \frac{1}{2} - x$
Symmetry operations

 For $(0,0,0)^+$ set

- | | | | |
|-------------------------|-------------------------|---------------------------------|---------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) 2 $0,y,\frac{1}{4}$ | (6) 2 $x,0,\frac{1}{4}$ | (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |
| (9) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (13) c $x,0,z$ | (14) c $0,y,z$ | (15) c x,\bar{x},z | (16) c x,x,z |

 For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})^+$ set

- | | | | |
|---|---|---|---|
| (1) $i(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ | (3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$ |
| (5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ | (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ | (7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$ | (8) 2 $x,\bar{x}+\frac{1}{2},0$ |
| (9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$ | (11) $\bar{4}^+$ $\frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$ | (12) $\bar{4}^-$ $0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$ |
| (13) a $x,\frac{1}{4},z$ | (14) b $\frac{1}{4},y,z$ | (15) m $x+\frac{1}{2},\bar{x},z$ | (16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z |

Maximal non-isomorphic subgroups (continued)

- IIa** [2] $P4_2/ncm$ (138) 1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4_2/mbc$ (135) 1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4_2/nbc$ (133) 1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4_2/mcm$ (132) 1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4/ncc$ (130) 1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4/mbm$ (127) 1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4/nbm$ (125) 1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
 [2] $P4/mcc$ (124) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16

IIb none

Maximal isomorphic subgroups of lowest index
IIc [3] $I4/mcm$ ($c' = 3c$) (140); [9] $I4/mcm$ ($a' = 3a, b' = 3b$) (140)

Minimal non-isomorphic supergroups
I [3] $Fm\bar{3}c$ (226)

II [2] $C4/mmm$ ($c' = \frac{1}{2}c$) ($P4/mmm$, 123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates (0,0,0)+ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				Reflection conditions
32 <i>m</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) x, y, \bar{z} (14) $\bar{x}, y, z + \frac{1}{2}$	(3) \bar{y}, x, z (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y, x, z + \frac{1}{2}$	General: $hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k, l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
16 <i>l</i> .. <i>m</i>	$x, x + \frac{1}{2}, z$ $\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	no extra conditions
16 <i>k</i> <i>m</i> ..	$x, y, 0$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, 0$ $y, x, \frac{1}{2}$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
16 <i>j</i> . 2 .	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x}, 0, \frac{1}{4}$ $x, 0, \frac{3}{4}$	$0, x, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$	$0, \bar{x}, \frac{1}{4}$ $0, x, \frac{3}{4}$	$hkl : l = 2n$
16 <i>i</i> .. 2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x, x, \frac{3}{4}$	$\bar{x}, x, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$	$x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$	$hkl : l = 2n$
8 <i>h</i> <i>m</i> . 2 <i>m</i>	$x, x + \frac{1}{2}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x, 0$	$x + \frac{1}{2}, \bar{x}, 0$	no extra conditions
8 <i>g</i> 2 . <i>mm</i>	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
8 <i>f</i> 4 . .	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$	$hkl : l = 2n$
8 <i>e</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : k, l = 2n$
4 <i>d</i> <i>m</i> . <i>mm</i>	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : l = 2n$
4 <i>c</i> 4/ <i>m</i> ..	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$
4 <i>b</i> $\bar{4}2m$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$			$hkl : l = 2n$
4 <i>a</i> 4 2 2	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$

Origin at 0,0,z

Along [100] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,0,0

Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,x,0

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4cm$ (108)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4/m11$ ($I4/m$, 87)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/m2/c1$ ($Ibam$, 72)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/m12/m$ ($Fmmm$, 69)	(1; 2; 7; 8; 9; 10; 15; 16)+

(Continued on preceding page)

$I4_1/amd$

D_{4h}^{19}

$4/mmm$

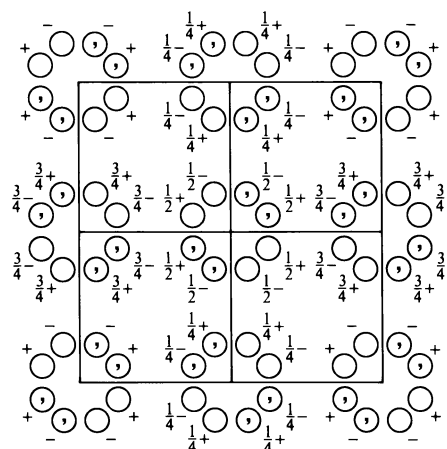
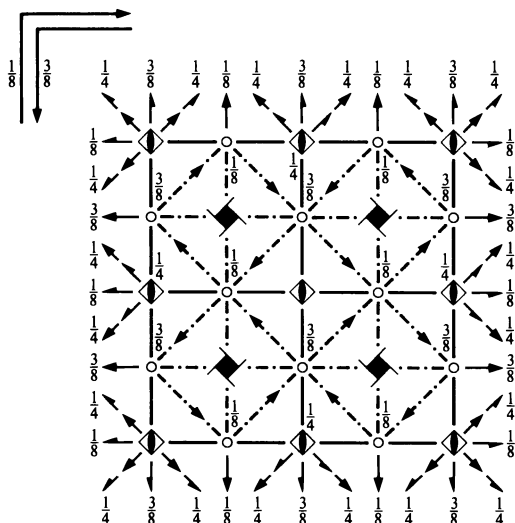
Tetragonal

No. 141

$I 4_1/a 2/m 2/d$

Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}m2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For $(0,0,0)^+$ set

- | | | | |
|---|--|--|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4}, -\frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, \frac{3}{8}$ | (6) 2 $x, \frac{1}{4}, \frac{1}{8}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x}, 0$ |
| (9) $\bar{1}$ $0, \frac{1}{4}, \frac{1}{8}$ | (10) a $x, y, \frac{3}{8}$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (14) m $0, y, z$ | (15) $d(\frac{1}{4}, -\frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{4}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $x - \frac{1}{4}, x, z$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|--|---|--|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, 0, z$ | (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{8}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, 0, \frac{3}{8}$ | (7) 2 $x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ $\frac{1}{4}, 0, \frac{3}{8}$ | (10) b $x, y, \frac{1}{8}$ | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) m $x, 0, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) $d(-\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{4}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{4}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	General:
32 <i>i</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$ (10) $x + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$ (11) y, \bar{x}, \bar{z} (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) \bar{x}, y, z (15) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (16) $y, x + \frac{1}{2}, z + \frac{1}{4}$	$hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
		Special: as above, plus
16 <i>h</i> . <i>m</i> .	$0, y, z$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{y}, \frac{1}{2}, z + \frac{1}{4}$ $y + \frac{1}{2}, 0, z + \frac{3}{4}$ $\frac{1}{2}, y, \bar{z} + \frac{3}{4}$ $0, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$ $y + \frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\bar{y}, 0, \bar{z}$	no extra conditions
16 <i>g</i> ..2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$ $x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n + 1$ or $2h + l = 4n$
16 <i>f</i> .2.	$x, \frac{1}{4}, \frac{1}{8}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{5}{8}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{8}$ $\frac{3}{4}, \bar{x}, \frac{7}{8}$ $\bar{x}, \frac{1}{4}, \frac{1}{8}$ $x + \frac{1}{2}, \frac{1}{4}, \frac{5}{8}$ $\frac{1}{4}, \bar{x}, \frac{7}{8}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{8}$	$hkl : l = 2n + 1$ or $h = 2n$
8 <i>e</i> 2 <i>m</i> <i>m</i> .	$0, 0, z$ $0, \frac{1}{2}, z + \frac{1}{4}$ $\frac{1}{2}, 0, \bar{z} + \frac{3}{4}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n + 1$ or $2h + l = 4n$
8 <i>d</i> .2/ <i>m</i> .	$0, \frac{1}{4}, \frac{5}{8}$ $\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$ $\frac{3}{4}, \frac{1}{2}, \frac{7}{8}$ $\frac{3}{4}, 0, \frac{3}{8}$ } 8 <i>c</i> .2/ <i>m</i> .	$hkl : l = 2n + 1$ or $h, k = 2n, h + k + l = 4n$
4 <i>b</i> $\bar{4}m2$	$0, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{3}{4}$ } 4 <i>a</i> $\bar{4}m2$	$hkl : l = 2n + 1$ or $2h + l = 4n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, \frac{3}{8}$

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4, md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4, 22$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4_1/a11$ ($I4_1/a$, 88)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/a2/m1$ ($Imma$, 74)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/a12/d$ ($Fddd$, 70)	(1; 2; 7; 8; 9; 10; 15; 16)+

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $I4_1/amd$ ($\mathbf{c}' = 3\mathbf{c}$) (141); [9] $I4_1/amd$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (141)**Minimal non-isomorphic supergroups****I** [3] $Fd\bar{3}m$ (227)**II** [2] $C4_2/amd$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4_2/nnm$, 134)

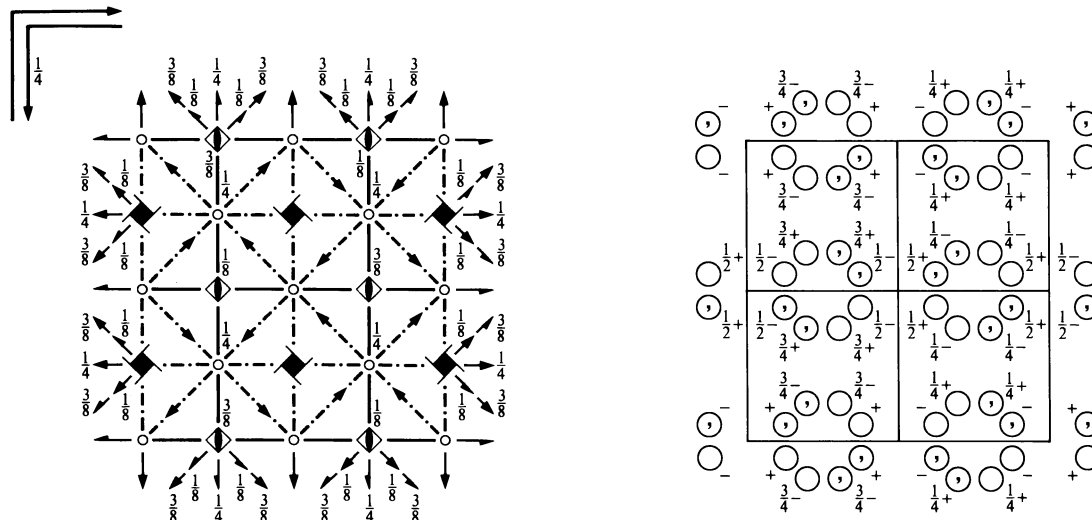
$I4_1/amd$ D_{4h}^{19} $4/mmm$

Tetragonal

No. 141

 $I 4_1/a 2/m 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2



Origin at centre $(2/m)$ at $b(2/m, 2/n)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For $(0, 0, 0)^+$ set

- | | | | |
|---|--|---|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $4^+(0, 0, \frac{1}{4})$ $-\frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{3}{4})$ $\frac{1}{4}, 0, z$ |
| (5) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (6) 2 $x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x + \frac{1}{4}, \frac{1}{8}$ | (8) 2 $x, \bar{x} + \frac{1}{4}, \frac{3}{8}$ |
| (9) $\bar{1}$ $0, 0, 0$ | (10) a $x, y, \frac{1}{4}$ | (11) 4^+ $\frac{1}{2}, -\frac{1}{4}, z; \frac{1}{2}, -\frac{1}{4}, \frac{3}{8}$ | (12) 4^- $0, \frac{3}{4}, z; 0, \frac{3}{4}, \frac{1}{8}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (14) m $0, y, z$ | (15) $d(\frac{1}{4}, -\frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{2}, \bar{x}, z$ | (16) $d(\frac{3}{4}, \frac{3}{4}, \frac{1}{4})$ x, x, z |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|---|---|---|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{3}{4})$ $\frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{4})$ $\frac{3}{4}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $0, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x - \frac{1}{4}, \frac{3}{8}$ | (8) 2 $x, \bar{x} + \frac{3}{4}, \frac{1}{8}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) b $x, y, 0$ | (11) 4^+ $\frac{1}{2}, \frac{1}{4}, z; \frac{1}{2}, \frac{1}{4}, \frac{1}{8}$ | (12) 4^- $0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$ |
| (13) m $x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) $d(-\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{2}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	General:
32 <i>i</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ (4) $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (6) x, \bar{y}, \bar{z} (7) $y + \frac{1}{4}, x + \frac{3}{4}, \bar{z} + \frac{1}{4}$ (8) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (11) $y + \frac{3}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (12) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, \bar{z} + \frac{1}{4}$ (13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (14) \bar{x}, y, z (15) $\bar{y} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ (16) $y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	$hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
16 <i>h</i> . <i>m</i> .	$0, y, z$ $\frac{1}{2}, \bar{y}, z + \frac{1}{2}$ $\bar{y} + \frac{1}{4}, \frac{3}{4}, z + \frac{1}{4}$ $y + \frac{1}{4}, \frac{1}{4}, z + \frac{3}{4}$ $\frac{1}{2}, y, \bar{z} + \frac{1}{2}$ $0, \bar{y}, \bar{z}$ $y + \frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{3}{4}$	no extra conditions
16 <i>g</i> ..2	$x, x + \frac{1}{4}, \frac{7}{8}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{3}{4}, \frac{3}{8}$ $\bar{x}, x + \frac{3}{4}, \frac{1}{8}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{4}, \frac{5}{8}$ $\bar{x}, \bar{x} + \frac{3}{4}, \frac{1}{8}$ $x + \frac{1}{2}, x + \frac{1}{4}, \frac{5}{8}$ $x, \bar{x} + \frac{1}{4}, \frac{7}{8}$ $\bar{x} + \frac{1}{2}, x + \frac{3}{4}, \frac{3}{8}$	$hkl : l = 2n + 1$ or $2h + l = 4n$
16 <i>f</i> .2.	$x, 0, 0$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{4}, x + \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{3}{4}$ $\bar{x}, 0, 0$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $\frac{3}{4}, \bar{x} + \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{3}{4}, \frac{1}{4}$	$hkl : l = 2n + 1$ or $h = 2n$
8 <i>e</i> 2 <i>m</i> <i>m</i> .	$0, \frac{1}{4}, z$ $0, \frac{3}{4}, z + \frac{1}{4}$ $\frac{1}{2}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{1}{4}$	$hkl : l = 2n + 1$ or $2h + l = 4n$
8 <i>d</i> .2/ <i>m</i> .	$0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ } 8 <i>c</i> .2/ <i>m</i> .	$hkl : l = 2n + 1$ or $h, k = 2n, h + k + l = 4n$
4 <i>b</i> $\bar{4}m2$	$0, \frac{1}{4}, \frac{3}{8}$ $0, \frac{3}{4}, \frac{5}{8}$ } 4 <i>a</i> $\bar{4}m2$	$hkl : l = 2n + 1$ or $2h + l = 4n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4}, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{4}, \frac{1}{8}$

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x + \frac{1}{4}, \frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4, md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4, 22$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4_1/a11$ ($I4_1/a, 88$)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/a2/m1$ ($Imma, 74$)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/a12/d$ ($Fddd, 70$)	(1; 2; 7; 8; 9; 10; 15; 16)+

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $I4_1/amd$ ($\mathbf{c}' = 3\mathbf{c}$) (141); [9] $I4_1/amd$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (141)**Minimal non-isomorphic supergroups****I** [3] $Fd\bar{3}m$ (227)**II** [2] $C4_2/amd$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4_2/nnm, 134$)

$I4_1/acd$

D_{4h}^{20}

$4/mmm$

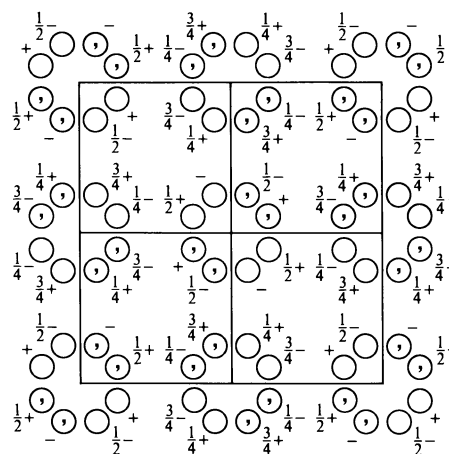
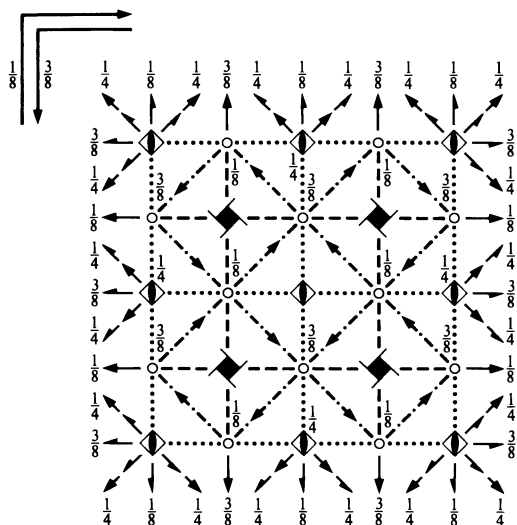
Tetragonal

No. 142

$I 4_1/a 2/c 2/d$

Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}c2_1$, at $0, \frac{1}{4}, -\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For $(0,0,0)^+$ set

- | | | | |
|---|--|--|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4}, -\frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, \frac{1}{8}$ | (6) 2 $x, \frac{1}{4}, \frac{3}{8}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}$ $0, \frac{1}{4}, \frac{1}{8}$ | (10) a $x, y, \frac{3}{8}$ | (11) 4^+ $0, 0, z; 0, 0, 0$ | (12) 4^- $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (13) a $x, \frac{1}{4}, z$ | (14) c $0, y, z$ | (15) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{4}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x - \frac{1}{4}, x, z$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|--|--|--|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, 0, z$ | (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0,\frac{1}{2},0)$ $0, y, \frac{3}{8}$ | (6) $2(\frac{1}{2},0,0)$ $x, 0, \frac{1}{8}$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, 0, \frac{3}{8}$ | (10) b $x, y, \frac{1}{8}$ | (11) 4^+ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (12) 4^- $0, 0, z; 0, 0, 0$ |
| (13) c $x, 0, z$ | (14) b $\frac{1}{4}, y, z$ | (15) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{4}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{4}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
32 <i>g</i> 1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{4}$ (9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$ (10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$ (14) $\bar{x},y,z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$ (11) y,\bar{x},\bar{z} (15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (16) $y,x+\frac{1}{2},z+\frac{3}{4}$	$hkl : h+k+l=2n$ $hk0 : h,k=2n$ $0kl : k,l=2n$ $hhl : 2h+l=4n$ $00l : l=4n$ $h00 : h=2n$ $h\bar{h}0 : h=2n$
16 <i>f</i> ..2	$x,x,\frac{1}{4}$ $\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$ $x+\frac{1}{2},x,\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$ $x,\bar{x},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},0$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$hkl : l=2n+1$ or $2h+l=4n$
16 <i>e</i> .2.	$\frac{1}{4},y,\frac{1}{8}$ $\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{8}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{5}{8}$ $\frac{3}{4},y,\frac{5}{8}$	$\bar{y},\frac{3}{4},\frac{3}{8}$ $y,\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},\frac{3}{4},\frac{7}{8}$ $\bar{y}+\frac{1}{2},\frac{3}{4},\frac{3}{8}$	$hkl : l=2n+1$ or $h=2n$
16 <i>d</i> 2..	$0,0,z$ $0,\frac{1}{2},\bar{z}+\frac{1}{4}$	$0,\frac{1}{2},z+\frac{1}{4}$ $0,0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$ $\frac{1}{2},0,z+\frac{1}{4}$	$hkl : 2h+l=4n$
16 <i>c</i> $\bar{1}$	$0,\frac{1}{4},\frac{1}{8}$ $\frac{1}{2},\frac{1}{4},\frac{5}{8}$ $\frac{3}{4},\frac{1}{2},\frac{3}{8}$ $\frac{3}{4},0,\frac{7}{8}$ $\frac{1}{2},\frac{1}{4},\frac{1}{8}$ $0,\frac{1}{4},\frac{5}{8}$ $\frac{3}{4},\frac{1}{2},\frac{7}{8}$ $\frac{3}{4},0,\frac{3}{8}$				$hkl : h,k=2n, h+k+l=4n$
8 <i>b</i> 2.22	$0,0,\frac{1}{4}$	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$0,0,\frac{3}{4}$	$hkl : 2h+l=4n$
8 <i>a</i> $\bar{4}$..	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},0$	$hkl : 2h+l=4n$

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ Origin at $0,0,z$ Along [100] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x,0,\frac{1}{8}$ Along [110] $c2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x,x,0$ **Maximal non-isomorphic subgroups**

I	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4,cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4,22$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4_1/a11$ ($I4_1/a$, 88)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/a2/c1$ ($Ibca$, 73)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/a12/d$ ($Fddd$, 70)	(1; 2; 7; 8; 9; 10; 15; 16)+

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $I4_1/acd$ ($\mathbf{c}' = 3\mathbf{c}$) (142); [9] $I4_1/acd$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (142)**Minimal non-isomorphic supergroups****I** [3] $Fd\bar{3}c$ (228); [3] $Ia\bar{3}d$ (230)**II** [2] $C4_2/amd$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4_2/nm$, 134)

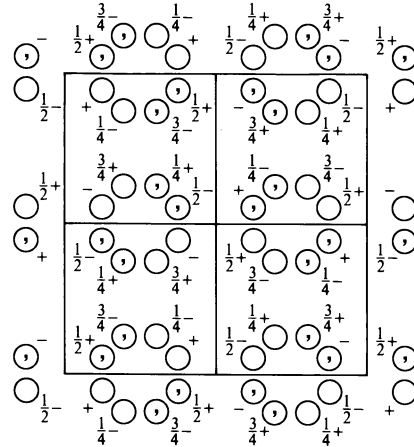
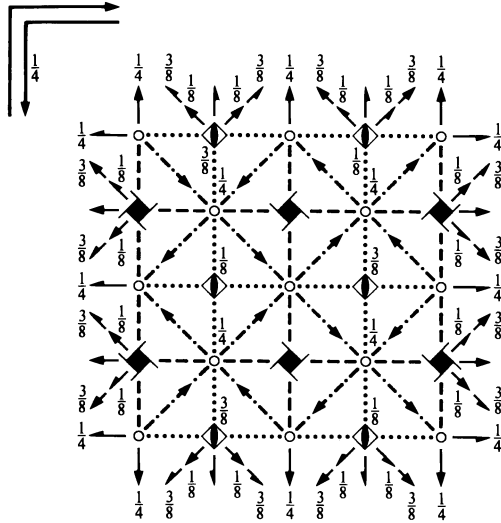
$I4_1/acd$ D_{4h}^{20} $4/mmm$

Tetragonal

No. 142

 $I 4_1/a 2/c 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $b(c,a)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}$ Asymmetric unit $0 \leq x \leq \frac{1}{2}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{8}$ **Symmetry operations**For $(0,0,0)+$ set

- | | | | |
|-----------------------------|--|---|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4}, 0, z$ |
| (5) 2 $\frac{1}{4}, y, 0$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x + \frac{1}{4}, \frac{3}{8}$ | (8) 2 $x, \bar{x} + \frac{1}{4}, \frac{1}{8}$ |
| (9) $\bar{1}$ $0, 0, 0$ | (10) a $x, y, \frac{1}{4}$ | (11) 4^+ $\frac{1}{2}, -\frac{1}{4}, z; \frac{1}{2}, -\frac{1}{4}, \frac{3}{8}$ | (12) 4^- $0, \frac{3}{4}, z; 0, \frac{3}{4}, \frac{1}{8}$ |
| (13) a $x, 0, z$ | (14) c $0, y, z$ | (15) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{2}, \bar{x}, z$ | (16) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ x, x, z |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|--|---|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x - \frac{1}{4}, \frac{1}{8}$ | (8) 2 $x, \bar{x} + \frac{3}{4}, \frac{3}{8}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) b $x, y, 0$ | (11) 4^+ $\frac{1}{2}, \frac{1}{4}, z; \frac{1}{2}, \frac{1}{4}, \frac{1}{8}$ | (12) 4^- $0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$ |
| (13) c $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{2}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:	
32 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ (7) $y + \frac{1}{4}, x + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (11) $y + \frac{3}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (15) $\bar{y} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{1}{4}$	(4) $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ (8) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (12) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, \bar{z} + \frac{1}{4}$ (16) $y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{3}{4}$	$hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k, l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$	
16 <i>f</i> ..2	$x, x + \frac{1}{4}, \frac{1}{8}$ $\bar{x}, \bar{x} + \frac{3}{4}, \frac{7}{8}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{3}{4}, \frac{5}{8}$ $x + \frac{1}{2}, x + \frac{1}{4}, \frac{3}{8}$	$\bar{x}, x + \frac{3}{4}, \frac{3}{8}$ $x, \bar{x} + \frac{1}{4}, \frac{5}{8}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{4}, \frac{7}{8}$ $\bar{x} + \frac{1}{2}, x + \frac{3}{4}, \frac{1}{8}$	$hkl : l = 2n + 1$ or $2h + l = 4n$	
16 <i>e</i> .2.	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, 0, \frac{3}{4}$ $x + \frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \bar{x} + \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \bar{x} + \frac{1}{4}, 0$ $\frac{3}{4}, x + \frac{3}{4}, 0$	$hkl : l = 2n + 1$ or $h = 2n$	
16 <i>d</i> 2..	$0, \frac{1}{4}, z$ $0, \frac{3}{4}, \bar{z}$	$0, \frac{3}{4}, z + \frac{1}{4}$ $0, \frac{1}{4}, \bar{z} + \frac{3}{4}$	$\frac{1}{2}, \frac{1}{4}, \bar{z}$ $\frac{1}{2}, \frac{3}{4}, z$	$\frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{3}{4}$ $\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}$	$hkl : 2h + l = 4n$	
16 <i>c</i> $\bar{1}$	0,0,0	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, 0, 0$ 0,0, $\frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h, k = 2n, h + k + l = 4n$
8 <i>b</i> 2.22	$0, \frac{1}{4}, \frac{1}{8}$	$0, \frac{3}{4}, \frac{3}{8}$	$0, \frac{3}{4}, \frac{7}{8}$	$0, \frac{1}{4}, \frac{5}{8}$	$hkl : 2h + l = 4n$	
8 <i>a</i> $\bar{4}$..	$0, \frac{1}{4}, \frac{3}{8}$	$0, \frac{3}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$	$hkl : 2h + l = 4n$	

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4}, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x + \frac{1}{4}, \frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4, cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4, 22$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4_1/a11$ ($I4_1/a, 88$)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/a2/c1$ ($Ibca, 73$)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/a12/d$ ($Fddd, 70$)	(1; 2; 7; 8; 9; 10; 15; 16)+

IIa none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3] $I4_1/acd$ ($\mathbf{c}' = 3\mathbf{c}$) (142); [9] $I4_1/acd$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (142)**Minimal non-isomorphic supergroups****I** [3] $Fd\bar{3}c$ (228); [3] $Ia\bar{3}d$ (230)**II** [2] $C4_2/amd$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4_2/nnm, 134$)

$P3$

C_3^1

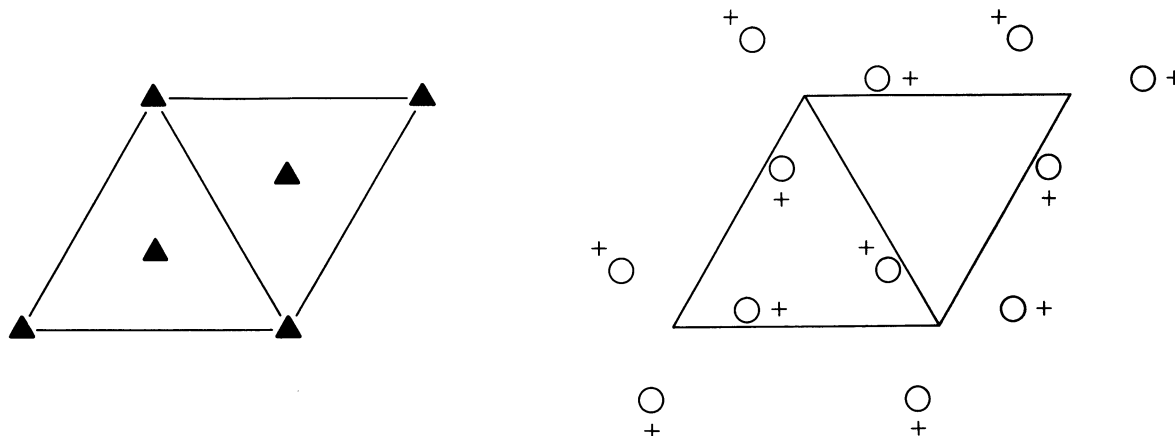
3

Trigonal

No. 143

$P3$

Patterson symmetry $P\bar{3}$



Origin on 3

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq 1$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, 1$ $\frac{1}{2}, 0, 1$ $\frac{2}{3}, \frac{1}{3}, 1$ $\frac{1}{3}, \frac{2}{3}, 1$ $0, \frac{1}{2}, 1$

Symmetry operations

(1) 1 (2) 3^+ $0, 0, z$ (3) 3^- $0, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
3 <i>d</i> 1	(1) x,y,z	(2) $\bar{y},x-y,z$	General: no conditions Special: no extra conditions
1 <i>c</i> 3..	$\frac{2}{3},\frac{1}{3},z$		
1 <i>b</i> 3..	$\frac{1}{3},\frac{2}{3},z$		
1 <i>a</i> 3..	$0,0,z$		

Symmetry of special projections

Along [001] $p3$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$	Along [100] $p1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$	Along [210] $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
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Maximal non-isomorphic subgroups

- I** [3] $P1(1)$ 1
IIa none
IIb [3] $P3_2(\mathbf{c}' = 3\mathbf{c})$ (145); [3] $P3_1(\mathbf{c}' = 3\mathbf{c})$ (144); [3] $R3(\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c})$ (146);
 [3] $R3(\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c})$ (146)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $P3(\mathbf{c}' = 2\mathbf{c})$ (143); [3] $H3(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})$ ($P3$, 143)

Minimal non-isomorphic supergroups

- I** [2] $P\bar{3}$ (147); [2] $P312$ (149); [2] $P321$ (150); [2] $P3m1$ (156); [2] $P31m$ (157); [2] $P3c1$ (158); [2] $P31c$ (159); [2] $P6$ (168);
 [2] $P6_3$ (173); [2] $P\bar{6}$ (174)
II [3] $R3$ (obverse) (146); [3] $R3$ (reverse) (146)

$P3_1$

C_3^2

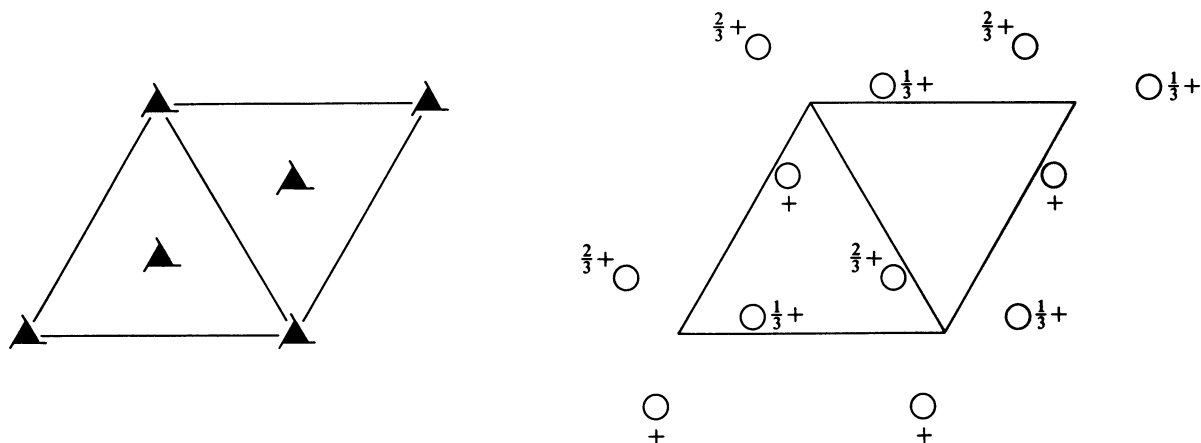
3

Trigonal

No. 144

$P3_1$

Patterson symmetry $P\bar{3}$



Origin on 3_1

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{3}$
 Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$
 $0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$ $0,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
3 <i>a</i> 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{1}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	General: $000l : l = 3n$

Symmetry of special projections

Along $[001]$ $p3$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$	Along $[100]$ $p1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$	Along $[210]$ $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
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Maximal non-isomorphic subgroups

- I $[3]P1(1)$ 1
- IIa none
- IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2]P3_2(\mathbf{c}' = 2\mathbf{c})(145)$; $[3]H3_1(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})(P3_1, 144)$; $[7]P3_1(\mathbf{c}' = 7\mathbf{c})(144)$

Minimal non-isomorphic supergroups

- I $[2]P3_1(12)(151)$; $[2]P3_1(21)(152)$; $[2]P6_1(169)$; $[2]P6_4(172)$
- II $[3]R3(\text{obverse})(146)$; $[3]R3(\text{reverse})(146)$; $[3]P3(\mathbf{c}' = \frac{1}{3}\mathbf{c})(143)$

Trigonal

3

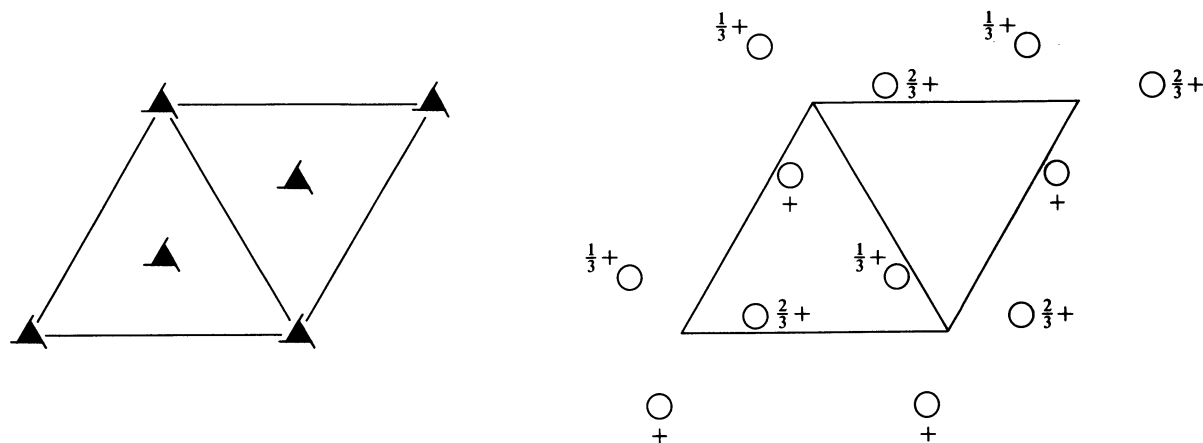
C_3^3

$P3_2$

Patterson symmetry $P\bar{3}$

$P3_2$

No. 145



Origin on 3_2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{3}$
 Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$
 $0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$ $0,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
3 <i>a</i> 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	General: $000l : l = 3n$

Symmetry of special projections

Along $[001]$ $p3$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$	Along $[100]$ $p1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$	Along $[210]$ $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,\frac{1}{2}x,0$
--	---	--

Maximal non-isomorphic subgroups

I $[3]P1(1)$ 1
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2]P3_2(\mathbf{c}' = 2\mathbf{c})(144)$; $[3]H3_2(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})(P3_2, 145)$; $[7]P3_2(\mathbf{c}' = 7\mathbf{c})(145)$

Minimal non-isomorphic supergroups

I $[2]P3_212(153)$; $[2]P3_221(154)$; $[2]P6_5(170)$; $[2]P6_2(171)$
II $[3]R3(\text{obverse})(146)$; $[3]R3(\text{reverse})(146)$; $[3]P3(\mathbf{c}' = \frac{1}{3}\mathbf{c})(143)$

$R\bar{3}$

C_3^4

3

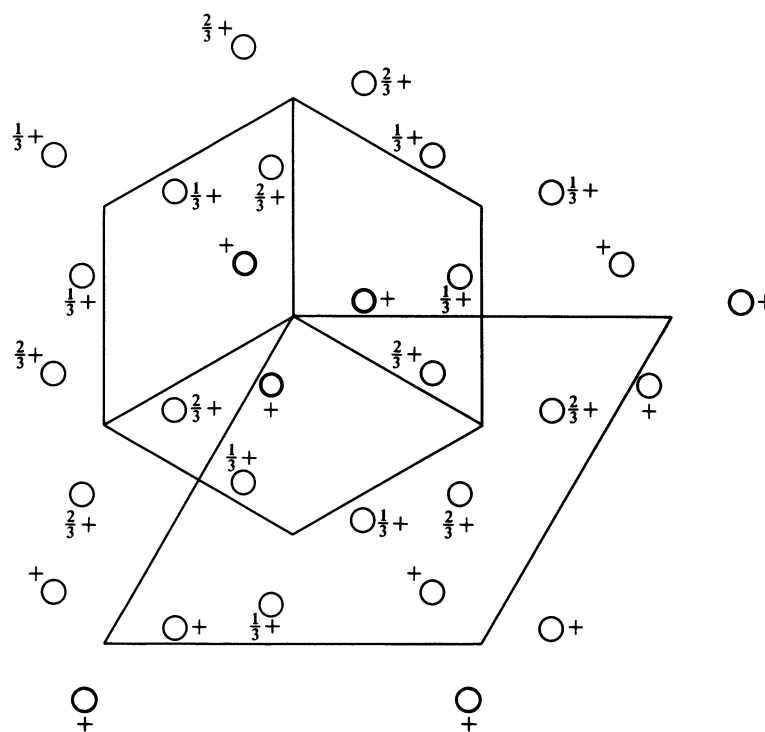
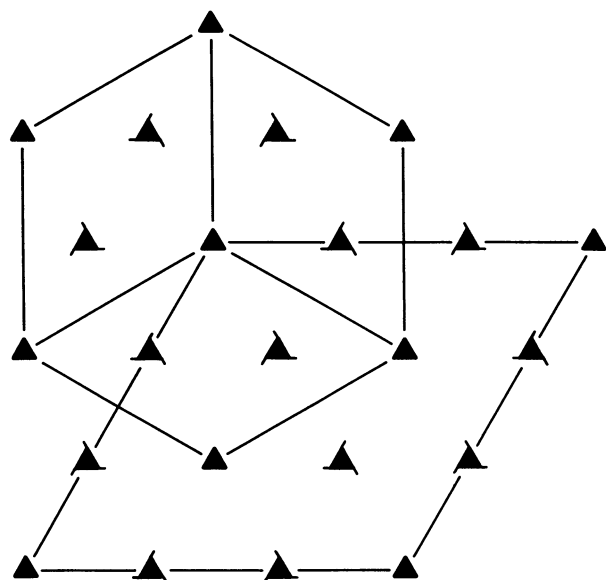
Trigonal

No. 146

$R\bar{3}$

Patterson symmetry $R\bar{3}$

HEXAGONAL AXES



Origin on 3

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{3}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$
Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{2}{3}, \frac{1}{3}, 0 \quad \frac{1}{3}, \frac{2}{3}, 0 \quad 0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{3} \quad \frac{1}{2}, 0, \frac{1}{3} \quad \frac{2}{3}, \frac{1}{3}, \frac{1}{3} \quad \frac{1}{3}, \frac{2}{3}, \frac{1}{3} \quad 0, \frac{1}{2}, \frac{1}{3}$

Symmetry operations

For $(0, 0, 0)+$ set

- (1) 1 (2) $3^+ 0, 0, z$ (3) $3^- 0, 0, z$

For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+$ set

- (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ (2) $3^+(0, 0, \frac{1}{3}) \quad \frac{1}{3}, \frac{1}{3}, z$ (3) $3^-(0, 0, \frac{1}{3}) \quad \frac{1}{3}, 0, z$

For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$ set

- (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ (2) $3^+(0, 0, \frac{2}{3}) \quad 0, \frac{1}{3}, z$ (3) $3^-(0, 0, \frac{2}{3}) \quad \frac{1}{3}, \frac{1}{3}, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+$ $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$

9 *b* 1 (1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$

Reflection conditions

General:

$$hkil : -h + k + l = 3n$$

$$hki0 : -h + k = 3n$$

$$hh\bar{2}hl : l = 3n$$

$$h\bar{h}0l : h + l = 3n$$

$$000l : l = 3n$$

$$h\bar{h}00 : h = 3n$$

Special: no extra conditions

3 *a* 3. 0,0,z

Symmetry of special projections

Along [001] $p3$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$$

Origin at 0,0,z

Along [100] $p1$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$$

Origin at $x, 0, 0$

Along [210] $p1$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{3}\mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [3] $R1 (P1, 1)$ 1+

IIa [3] $P3_2 (145)$ 1; $2 + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$; $3 + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$

[3] $P3_1 (144)$ 1; $2 + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; $3 + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$

[3] $P3 (143)$ 1; 2; 3

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $R3 (\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (146)$; [4] $R3 (\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}) (146)$

Minimal non-isomorphic supergroups

I [2] $R\bar{3} (148)$; [2] $R32 (155)$; [2] $R3m (160)$; [2] $R3c (161)$; [4] $P23 (195)$; [4] $F23 (196)$; [4] $I23 (197)$; [4] $P2_13 (198)$; [4] $I2_13 (199)$

II [3] $P3 (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}) (143)$

$R\bar{3}$ C_3^4

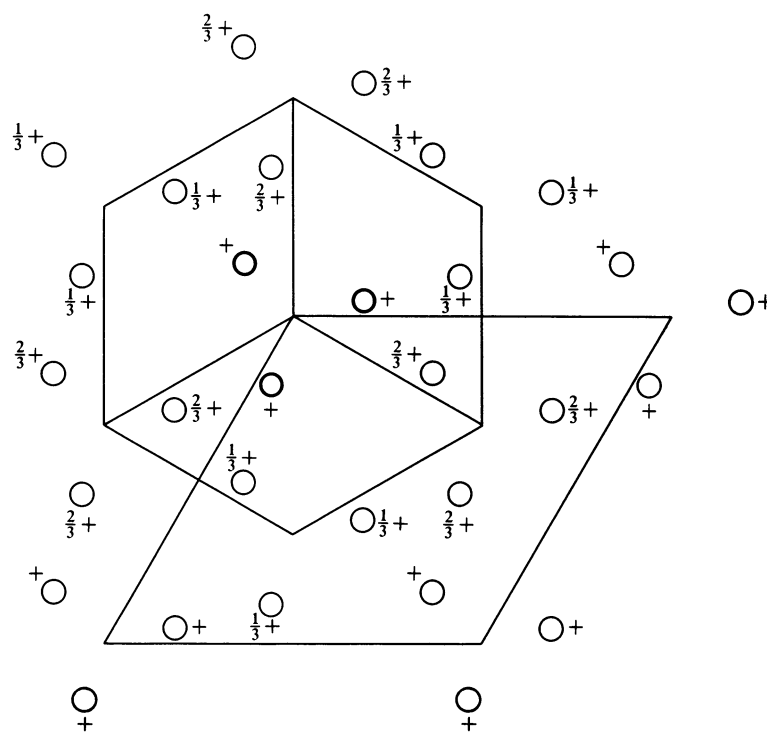
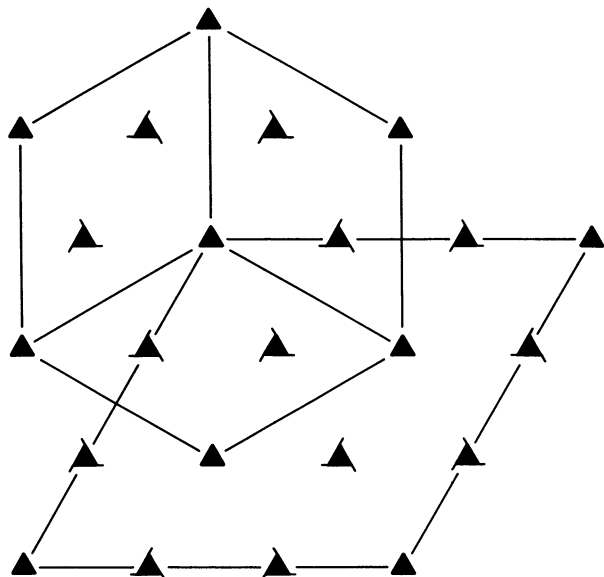
3

Trigonal

No. 146

 $R\bar{3}$ Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin on 3**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1; z \leq \min(x, y)$ Vertices $0, 0, 0 \quad 1, 0, 0 \quad 1, 1, 0 \quad 0, 1, 0 \quad 1, 1, 1$ **Symmetry operations**(1) 1 (2) $3^+ x, x, x$ (3) $3^- x, x, x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

3 b 1 (1) x,y,z (2) z,x,y (3) y,z,x

General:

no conditions

Special: no extra conditions

1 a 3. x,x,x

Symmetry of special projections

Along $[111] p3$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x,x,x

Along $[1\bar{1}0] p1$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \bar{x}, 0$

Along $[2\bar{1}\bar{1}] p1$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$$

Origin at $2x, \bar{x}, \bar{x}$

Maximal non-isomorphic subgroups

I [3] $R1 (P1, 1)$ 1

IIa none

IIb [3] $P3_2 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c})$ (145); [3] $P3_1 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c})$ (144);
[3] $P3 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c})$ (143)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3 (\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b})$ (146); [4] $R3 (\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c})$ (146)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198);
[4] $I2_13$ (199)

II [3] $P3 (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c}))$ (143)

$P\bar{3}$

C_{3i}^1

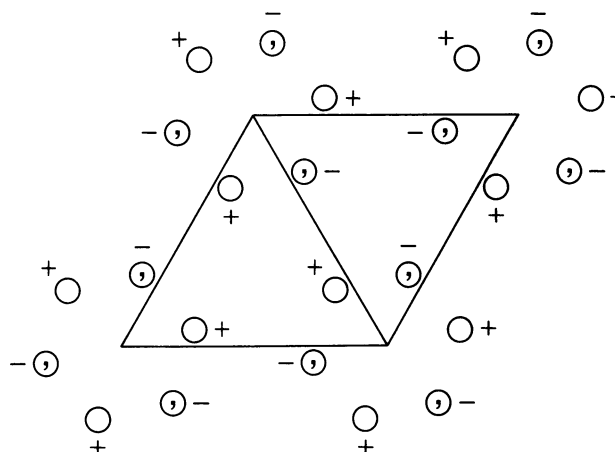
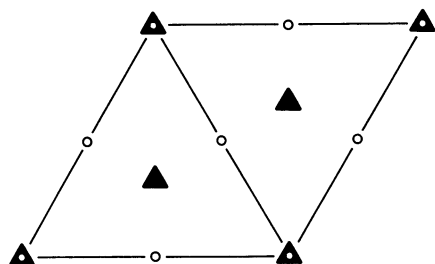
$\bar{3}$

Trigonal

No. 147

$P\bar{3}$

Patterson symmetry $P\bar{3}$



Origin at centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1 (2) 3^+ $0, 0, z$ (3) 3^- $0, 0, z$
 (4) $\bar{1}$ $0, 0, 0$ (5) $\bar{3}^+$ $0, 0, z$; $0, 0, 0$ (6) $\bar{3}^-$ $0, 0, z$; $0, 0, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions	
6	g	1	(1) x, y, z (4) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, \bar{z}$	General: no conditions Special: no extra conditions
3	f	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
3	e	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	
2	d	$3..$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$		
2	c	$3..$	$0, 0, z$	$0, 0, \bar{z}$		
1	b	$\bar{3}..$	$0, 0, \frac{1}{2}$			
1	a	$\bar{3}..$	$0, 0, 0$			

Symmetry of special projections

Along $[001]$ $p6$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p2$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[210]$ $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I $[2]P\bar{3}(143)$ 1; 2; 3
 $[3]P\bar{1}(2)$ 1; 4

IIa none

IIb $[3]R\bar{3}(\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c})(148)$; $[3]R\bar{3}(\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c})(148)$

Maximal isomorphic subgroups of lowest index

IIc $[2]P\bar{3}(\mathbf{c}' = 2\mathbf{c})(147)$; $[3]H\bar{3}(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})(P\bar{3}, 147)$

Minimal non-isomorphic supergroups

I $[2]P\bar{3}1m(162)$; $[2]P\bar{3}1c(163)$; $[2]P\bar{3}m1(164)$; $[2]P\bar{3}c1(165)$; $[2]P6/m(175)$; $[2]P6_3/m(176)$

II $[3]R\bar{3}(\text{obverse})(148)$; $[3]R\bar{3}(\text{reverse})(148)$

$R\bar{3}$
 C_{3i}^2
 $\bar{3}$

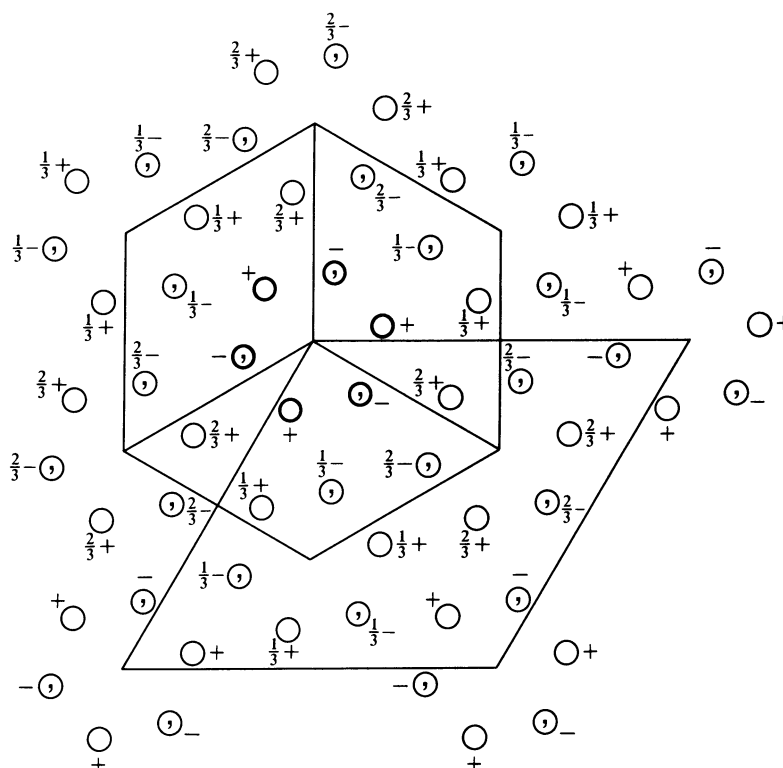
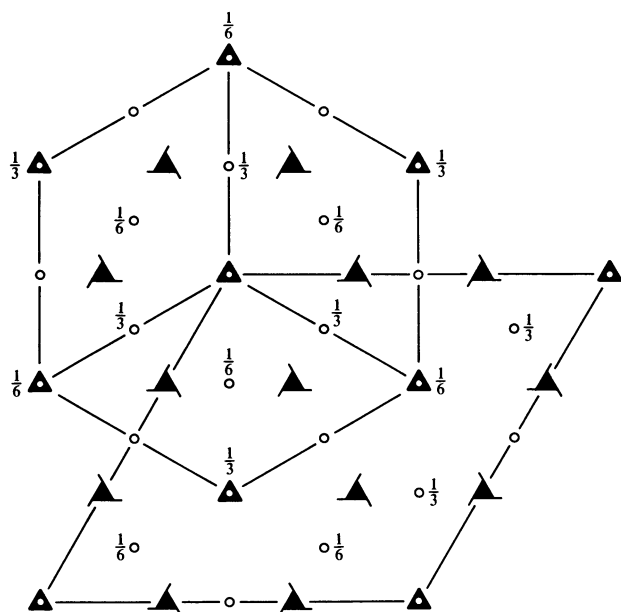
Trigonal

No. 148

 $R\bar{3}$

 Patterson symmetry $R\bar{3}$

HEXAGONAL AXES


 Origin at centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{6}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$
 Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{6}$ $\frac{1}{2}, 0, \frac{1}{6}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{6}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ $0, \frac{1}{2}, \frac{1}{6}$

Symmetry operations

 For $(0, 0, 0)^+$ set

- | | | |
|-----------------------|----------------------------------|----------------------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $\bar{1} 0, 0, 0$ | (5) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (6) $\bar{3}^- 0, 0, z; 0, 0, 0$ |

 For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})^+$ set

- | | | |
|---|--|--|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ | (2) $3^+(0, 0, \frac{1}{3}) \frac{1}{3}, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{1}{3}) \frac{1}{3}, 0, z$ |
| (4) $\bar{1} \frac{1}{3}, \frac{1}{6}, \frac{1}{6}$ | (5) $\bar{3}^+ \frac{1}{3}, -\frac{1}{3}, z; \frac{1}{3}, -\frac{1}{3}, \frac{1}{6}$ | (6) $\bar{3}^- \frac{1}{3}, \frac{2}{3}, z; \frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ |

 For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})^+$ set

- | | | |
|---|--|--|
| (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ | (2) $3^+(0, 0, \frac{2}{3}) 0, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{2}{3}) \frac{1}{3}, \frac{1}{3}, z$ |
| (4) $\bar{1} \frac{1}{6}, \frac{1}{3}, \frac{1}{3}$ | (5) $\bar{3}^+ \frac{2}{3}, \frac{1}{3}, z; \frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ | (6) $\bar{3}^- -\frac{1}{3}, \frac{1}{3}, z; -\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2); (4)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+ (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+ (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$

Reflection conditions

General:

18 f 1 (1) x, y, z (2) $\bar{y}, x-y, z$ (3) $\bar{x}+y, \bar{x}, z$
(4) $\bar{x}, \bar{y}, \bar{z}$ (5) $y, \bar{x}+y, \bar{z}$ (6) $x-y, x, \bar{z}$

$hkil$: $-h+k+l=3n$
 $hki0$: $-h+k=3n$
 $hh\bar{2}hl$: $l=3n$
 $h\bar{h}0l$: $h+l=3n$
 $000l$: $l=3n$
 $h\bar{h}00$: $h=3n$

Special: no extra conditions

9 e $\bar{1}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$

9 d $\bar{1}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

6 c $3.$ $0, 0, z$ $0, 0, \bar{z}$

3 b $\bar{3}.$ $0, 0, \frac{1}{2}$

3 a $\bar{3}.$ $0, 0, 0$

Symmetry of special projectionsAlong $[001]$ $p6$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$ Origin at $0, 0, z$ Along $[100]$ $p2$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$ Origin at $x, 0, 0$ Along $[210]$ $p2$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$ **Maximal non-isomorphic subgroups****I** $[2]R\bar{3}$ (146) (1; 2; 3)+ $[3]R\bar{1}$ ($P\bar{1}$, 2) (1; 4)+

IIa $\left\{ \begin{array}{l} [3]P\bar{3}$ (147) 1; 2; 3; 4; 5; 6
 $[3]P\bar{3}$ (147) 1; 2; 3; (4; 5; 6) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
 $[3]P\bar{3}$ (147) 1; 2; 3; (4; 5; 6) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ \end{array} \right.

IIb none**Maximal isomorphic subgroups of lowest index****IIc** $[2]R\bar{3}$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (148); $[4]R\bar{3}$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (148)**Minimal non-isomorphic supergroups****I** $[2]R\bar{3}m$ (166); $[2]R\bar{3}c$ (167); $[4]Pm\bar{3}$ (200); $[4]Pn\bar{3}$ (201); $[4]Fm\bar{3}$ (202); $[4]Fd\bar{3}$ (203); $[4]Im\bar{3}$ (204); $[4]Pa\bar{3}$ (205); $[4]Ia\bar{3}$ (206)**II** $[3]P\bar{3}$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (147)

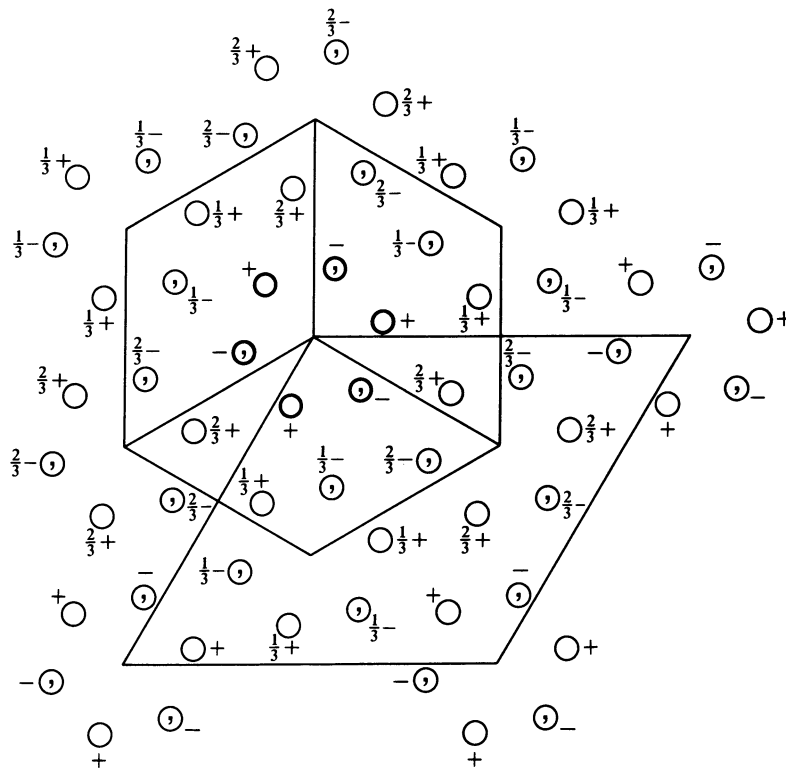
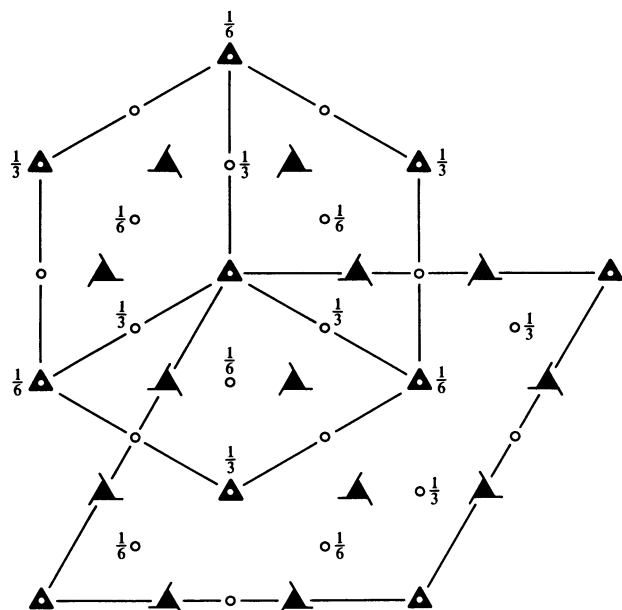
$R\bar{3}$ C_{3i}^2 $\bar{3}$

Trigonal

No. 148

 $R\bar{3}$ Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin at centre ($\bar{3}$)**Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}; z \leq \min(x, y, 1-x, 1-y)$ Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ **Symmetry operations**

- | | | |
|-------------------------|------------------------------------|------------------------------------|
| (1) 1 | (2) 3^+ x, x, x | (3) 3^- x, x, x |
| (4) $\bar{1}$ $0, 0, 0$ | (5) $\bar{3}^+$ $x, x, x; 0, 0, 0$ | (6) $\bar{3}^-$ $x, x, x; 0, 0, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 f 1	(1) x, y, z (4) $\bar{x}, \bar{y}, \bar{z}$	(2) z, x, y (5) $\bar{z}, \bar{x}, \bar{y}$	(3) y, z, x (6) $\bar{y}, \bar{z}, \bar{x}$	General: no conditions Special: no extra conditions
3 e $\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	
3 d $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$	
2 c 3.	x, x, x	$\bar{x}, \bar{x}, \bar{x}$		
1 b $\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
1 a $\bar{3}$.	$0, 0, 0$			

Symmetry of special projections

Along $[111] p6$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[1\bar{1}0] p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \bar{x}, 0$

Along $[2\bar{1}\bar{1}] p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$$

Origin at $2x, \bar{x}, \bar{x}$

Maximal non-isomorphic subgroups

I [2] $R\bar{3}$ (146) 1; 2; 3
[3] $R\bar{1}$ ($P\bar{1}, 2$) 1; 4

IIa none

IIb [3] $P\bar{3}$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$) (147)

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}$ ($\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b}$) (148); [4] $R\bar{3}$ ($\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}$) (148)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $Pm\bar{3}$ (200); [4] $Pn\bar{3}$ (201); [4] $Fm\bar{3}$ (202); [4] $Fd\bar{3}$ (203); [4] $Im\bar{3}$ (204); [4] $Pa\bar{3}$ (205); [4] $Ia\bar{3}$ (206)

II [3] $P\bar{3}$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$) (147)

$P312$

D_3^1

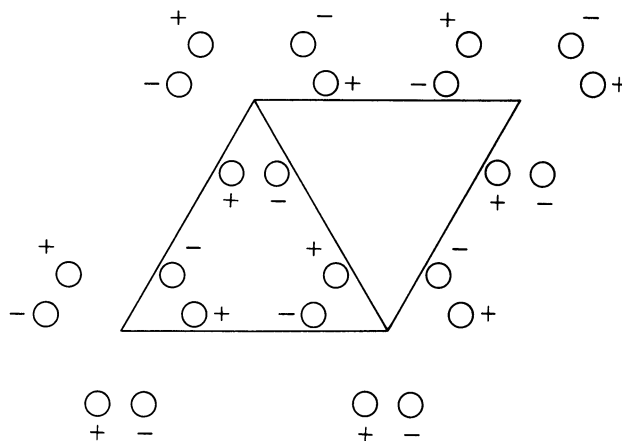
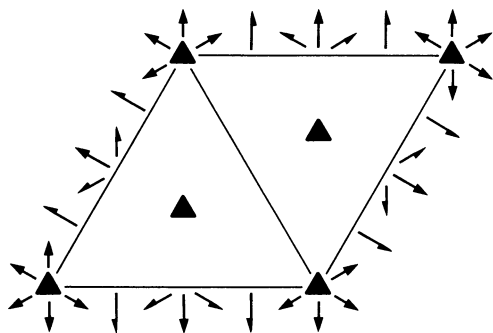
312

Trigonal

No. 149

$P312$

Patterson symmetry $P\bar{3}1m$



Origin at 312

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1 (2) $3^+ 0, 0, z$ (3) $3^- 0, 0, z$
 (4) 2 $x, \bar{x}, 0$ (5) 2 $x, 2x, 0$ (6) 2 $2x, x, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6	<i>l</i> 1	(1) x, y, z (4) $\bar{y}, \bar{x}, \bar{z}$	(2) $\bar{y}, x - y, z$ (5) $\bar{x} + y, y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x, x - y, \bar{z}$	General: no conditions Special: no extra conditions
3	<i>k</i> .. 2	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	
3	<i>j</i> .. 2	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	
2	<i>i</i> 3..	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$		
2	<i>h</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$		
2	<i>g</i> 3..	$0, 0, z$	$0, 0, \bar{z}$		
1	<i>f</i> 3.2	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$			
1	<i>e</i> 3.2	$\frac{2}{3}, \frac{1}{3}, 0$			
1	<i>d</i> 3.2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$			
1	<i>c</i> 3.2	$\frac{1}{3}, \frac{2}{3}, 0$			
1	<i>b</i> 3.2	$0, 0, \frac{1}{2}$			
1	<i>a</i> 3.2	$0, 0, 0$			

Symmetry of special projections

Along [001] $p3m1$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p11m$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3, 143$) 1; 2; 3
 { [3] $P112$ ($C2, 5$) 1; 4
 [3] $P112$ ($C2, 5$) 1; 5
 [3] $P112$ ($C2, 5$) 1; 6

IIa none

IIb [3] $P3_212$ ($\mathbf{c}' = 3\mathbf{c}$) (153); [3] $P3_112$ ($\mathbf{c}' = 3\mathbf{c}$) (151); [3] $H312$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P321, 150$);
 [3] $R32$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (155); [3] $R32$ ($\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (155)

Maximal isomorphic subgroups of lowest index

IIc [2] $P312$ ($\mathbf{c}' = 2\mathbf{c}$) (149); [4] $P312$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (149)

Minimal non-isomorphic supergroups

I [2] $P\bar{3}1m$ (162); [2] $P\bar{3}1c$ (163); [2] $P622$ (177); [2] $P6_322$ (182); [2] $P\bar{6}m2$ (187); [2] $P\bar{6}c2$ (188)

II [3] $H312$ ($P321, 150$)

$P321$

D_3^2

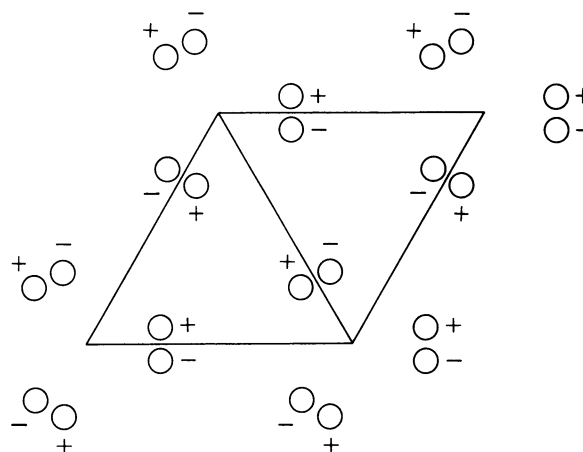
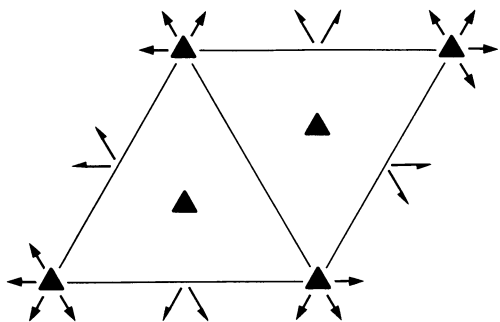
321

Trigonal

No. 150

$P321$

Patterson symmetry $P\bar{3}m1$



Origin at 321

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1 (2) 3^+ $0, 0, z$ (3) 3^- $0, 0, z$
 (4) 2 $x, x, 0$ (5) 2 $x, 0, 0$ (6) 2 $0, y, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6 <i>g</i> 1	(1) x, y, z (4) y, x, \bar{z}	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, \bar{z}$		General: no conditions Special: no extra conditions
3 <i>f</i> .2.	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$		
3 <i>e</i> .2.	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$		
2 <i>d</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$			
2 <i>c</i> 3..	$0, 0, z$	$0, 0, \bar{z}$			
1 <i>b</i> 32.	$0, 0, \frac{1}{2}$				
1 <i>a</i> 32.	$0, 0, 0$				

Symmetry of special projections

Along [001] $p31m$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3, 143$) 1; 2; 3
 { [3] $P121$ ($C2, 5$) 1; 4
 [3] $P121$ ($C2, 5$) 1; 5
 [3] $P121$ ($C2, 5$) 1; 6

IIa none

IIb [3] $P3_221$ ($\mathbf{c}' = 3\mathbf{c}$) (154); [3] $P3_121$ ($\mathbf{c}' = 3\mathbf{c}$) (152); [3] $H321$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P312, 149$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P321$ ($\mathbf{c}' = 2\mathbf{c}$) (150); [4] $P321$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (150)

Minimal non-isomorphic supergroups

I [2] $P\bar{3}m1$ (164); [2] $P\bar{3}c1$ (165); [2] $P622$ (177); [2] $P6_322$ (182); [2] $P\bar{6}2m$ (189); [2] $P\bar{6}2c$ (190)

II [3] $H321$ ($P312, 149$); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155)

$P3_112$

D_3^3

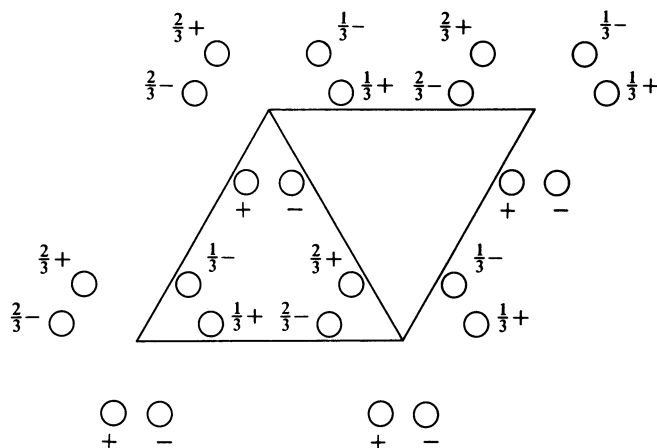
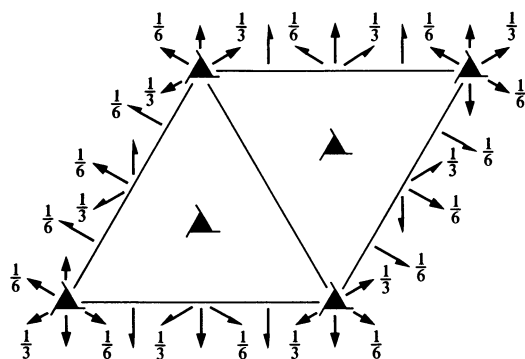
312

Trigonal

No. 151

$P3_112$

Patterson symmetry $P\bar{3}1m$



Origin on $2[210]$ at $3_11(1,1,2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$
 Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$
 $0,0,\frac{1}{6}$ $1,0,\frac{1}{6}$ $1,1,\frac{1}{6}$ $0,1,\frac{1}{6}$

Symmetry operations

- (1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
 (4) 2 $x,\bar{x},\frac{1}{3}$ (5) 2 $x,2x,\frac{1}{6}$ (6) 2 $2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>c</i> 1	(1) x, y, z (4) $\bar{y}, \bar{x}, \bar{z} + \frac{2}{3}$	(2) $\bar{y}, x - y, z + \frac{1}{3}$ (5) $\bar{x} + y, y, \bar{z} + \frac{1}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$ (6) $x, x - y, \bar{z}$	$000l : l = 3n$
				Special: no extra conditions
3 <i>b</i> .. 2	$x, \bar{x}, \frac{5}{6}$	$x, 2x, \frac{1}{6}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>a</i> .. 2	$x, \bar{x}, \frac{1}{3}$	$x, 2x, \frac{2}{3}$	$2\bar{x}, \bar{x}, 0$	

Symmetry of special projections

Along [001] $p3m1$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at 0, 0, z

Along [100] $p11m$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, \frac{1}{6}$

Along [210] $p2$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P3_111$ ($P3_1, 144$)	1; 2; 3
	{ [3] $P112$ ($C2, 5$)	1; 4
	{ [3] $P112$ ($C2, 5$)	1; 5
	{ [3] $P112$ ($C2, 5$)	1; 6

IIa none

IIb [3] $H3_112$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3, 21, 152$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_212$ ($\mathbf{c}' = 2\mathbf{c}$) (153); [4] $P3_112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (151); [7] $P3_112$ ($\mathbf{c}' = 7\mathbf{c}$) (151)

Minimal non-isomorphic supergroups

I [2] $P6_122$ (178); [2] $P6_422$ (181)

II [3] $H3_112$ ($P3_121, 152$); [3] $P312$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (149)

$P3_121$

D_3^4

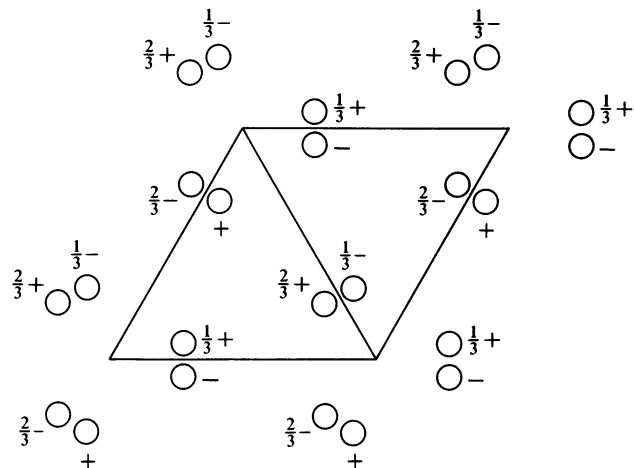
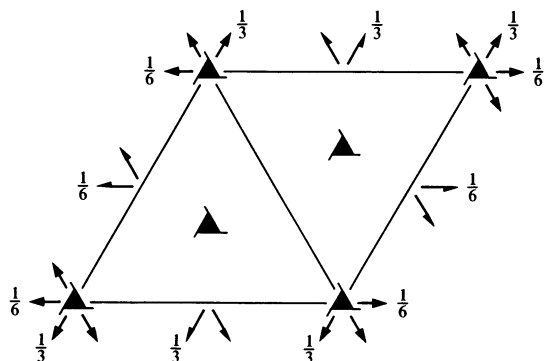
321

Trigonal

No. 152

$P3_121$

Patterson symmetry $P\bar{3}m1$



Origin on $2[110]$ at $3_1(1,1,2)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

- (1) 1 (2) $3^+(0,0,\frac{1}{3}) \quad 0,0,z$ (3) $3^-(0,0,\frac{2}{3}) \quad 0,0,z$
 (4) 2 $x,x,0$ (5) 2 $x,0,\frac{1}{3}$ (6) 2 $0,y,\frac{1}{6}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>c</i> 1	(1) x, y, z (4) y, x, \bar{z}	(2) $\bar{y}, x - y, z + \frac{1}{3}$ (5) $x - y, \bar{y}, \bar{z} + \frac{2}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$ (6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{3}$	$000l : l = 3n$
				Special: no extra conditions
3 <i>b</i> .2.	$x, 0, \frac{5}{6}$	$0, x, \frac{1}{6}$	$\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>a</i> .2.	$x, 0, \frac{1}{3}$	$0, x, \frac{2}{3}$	$\bar{x}, \bar{x}, 0$	

Symmetry of special projections

Along [001] $p31m$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at 0, 0, z

Along [100] $p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, \frac{1}{3}$

Along [210] $p11m$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{2}x, \frac{1}{6}$

Maximal non-isomorphic subgroups

I	[2] $P3_111$ ($P3_1, 144$)	1; 2; 3	
	{	[3] $P121$ ($C2, 5$)	1; 4
		[3] $P121$ ($C2, 5$)	1; 5
		[3] $P121$ ($C2, 5$)	1; 6

IIa none

IIb [3] $H3_121$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3, 12, 151$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_221$ ($\mathbf{c}' = 2\mathbf{c}$) (154); [4] $P3_121$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (152); [7] $P3_121$ ($\mathbf{c}' = 7\mathbf{c}$) (152)

Minimal non-isomorphic supergroups

I [2] $P6_122$ (178); [2] $P6_422$ (181)

II [3] $H3_121$ ($P3_1, 12, 151$); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155); [3] $P321$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (150)

$P3_212$

D_3^5

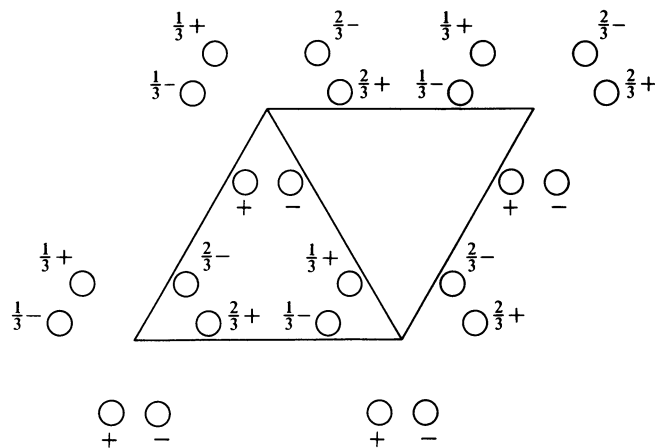
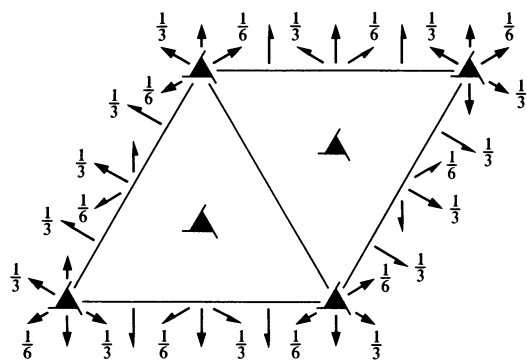
312

Trigonal

No. 153

$P3_212$

Patterson symmetry $P\bar{3}1m$



Origin on $2[210]$ at $3_21(1,1,2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$
 Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$
 $0,0,\frac{1}{6}$ $1,0,\frac{1}{6}$ $1,1,\frac{1}{6}$ $0,1,\frac{1}{6}$

Symmetry operations

- (1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
 (4) 2 $x,\bar{x},\frac{1}{6}$ (5) 2 $x,2x,\frac{1}{3}$ (6) 2 $2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 <i>c</i> 1	(1) x, y, z (4) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{3}$	(2) $\bar{y}, x - y, z + \frac{2}{3}$ (5) $\bar{x} + y, y, \bar{z} + \frac{2}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$ (6) $x, x - y, \bar{z}$	General: $000l : l = 3n$ Special: no extra conditions
3 <i>b</i> .. 2	$x, \bar{x}, \frac{1}{6}$	$x, 2x, \frac{5}{6}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>a</i> .. 2	$x, \bar{x}, \frac{2}{3}$	$x, 2x, \frac{1}{3}$	$2\bar{x}, \bar{x}, 0$	

Symmetry of special projections

Along [001] $P3m1$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at 0, 0, z

Along [100] $P11m$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, \frac{1}{3}$

Along [210] $P2$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P3_211$ ($P3_2, 145$)	1; 2; 3
	{ [3] $P112$ ($C2, 5$)	1; 4
	{ [3] $P112$ ($C2, 5$)	1; 5
	{ [3] $P112$ ($C2, 5$)	1; 6

IIa none

IIb [3] $H3_212$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3_221, 154$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_112$ ($\mathbf{c}' = 2\mathbf{c}$) (151); [4] $P3_212$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (153); [7] $P3_212$ ($\mathbf{c}' = 7\mathbf{c}$) (153)

Minimal non-isomorphic supergroups

I [2] $P6_522$ (179); [2] $P6_222$ (180)

II [3] $H3_212$ ($P3_221, 154$); [3] $P312$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (149)

$P3_221$

D_3^6

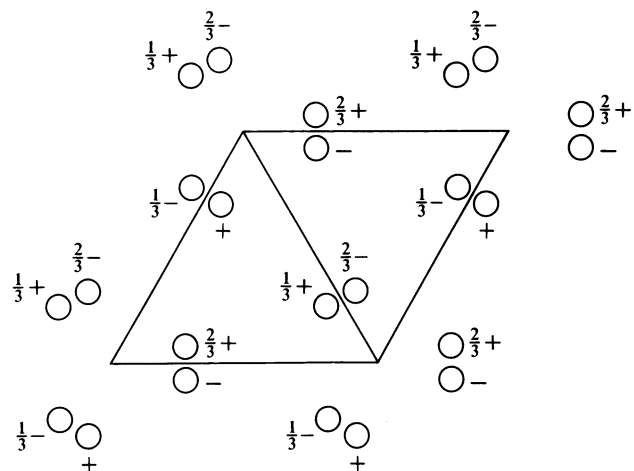
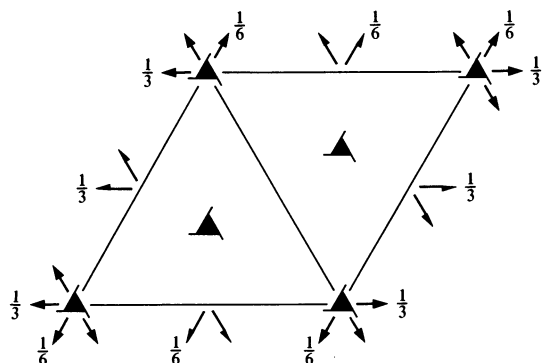
321

Trigonal

No. 154

$P3_221$

Patterson symmetry $P\bar{3}m1$



Origin on $2[110]$ at $3_2(1,1,2)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$

$0,0,\frac{1}{6}$ $1,0,\frac{1}{6}$ $1,1,\frac{1}{6}$ $0,1,\frac{1}{6}$

Symmetry operations

- (1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
 (4) 2 $x,x,0$ (5) 2 $x,0,\frac{1}{6}$ (6) 2 $0,y,\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>c</i> 1	(1) x, y, z (4) y, x, \bar{z}	(2) $\bar{y}, x - y, z + \frac{2}{3}$ (5) $x - y, \bar{y}, \bar{z} + \frac{1}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$ (6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{2}{3}$	$000l : l = 3n$
				Special: no extra conditions
3 <i>b</i> .2.	$x, 0, \frac{1}{6}$	$0, x, \frac{5}{6}$	$\bar{x}, \bar{x}, \frac{1}{2}$	
3 <i>a</i> .2.	$x, 0, \frac{2}{3}$	$0, x, \frac{1}{3}$	$\bar{x}, \bar{x}, 0$	

Symmetry of special projections

Along [001] $p31m$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at $0, 0, z$

Along [100] $p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, \frac{1}{6}$

Along [210] $p11m$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \frac{1}{2}x, \frac{1}{3}$

Maximal non-isomorphic subgroups

I	[2] $P3_211$ ($P3_2, 145$)	1; 2; 3
	{ [3] $P121$ ($C2, 5$)	1; 4
	{ [3] $P121$ ($C2, 5$)	1; 5
	{ [3] $P121$ ($C2, 5$)	1; 6

IIa none

IIb [3] $H3_221$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3_212, 153$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_121$ ($\mathbf{c}' = 2\mathbf{c}$) (152); [4] $P3_221$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (154); [7] $P3_221$ ($\mathbf{c}' = 7\mathbf{c}$) (154)

Minimal non-isomorphic supergroups

I [2] $P6_522$ (179); [2] $P6_222$ (180)

II [3] $H3_221$ ($P3_212, 153$); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155); [3] $P321$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (150)

$R32$

D_3^7

32

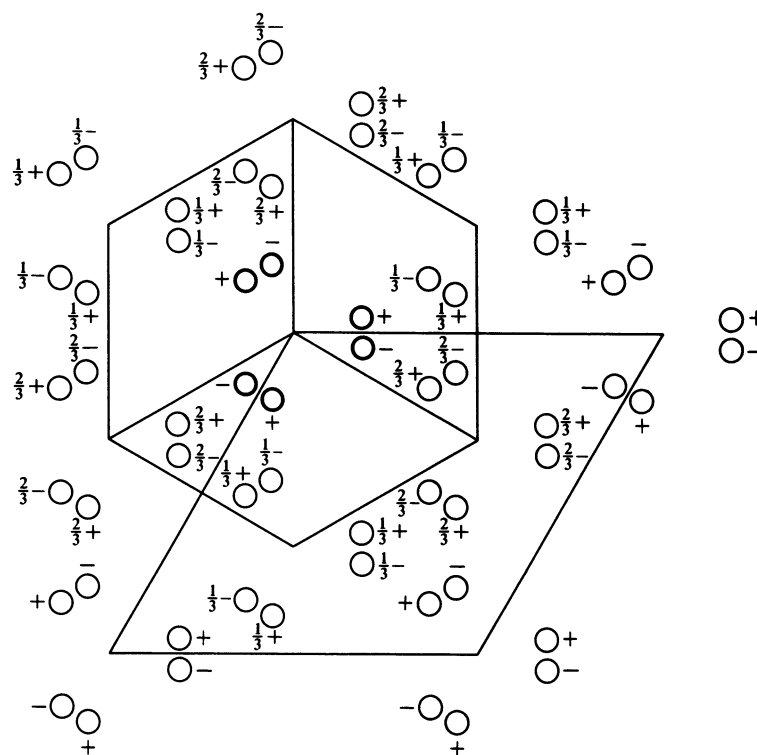
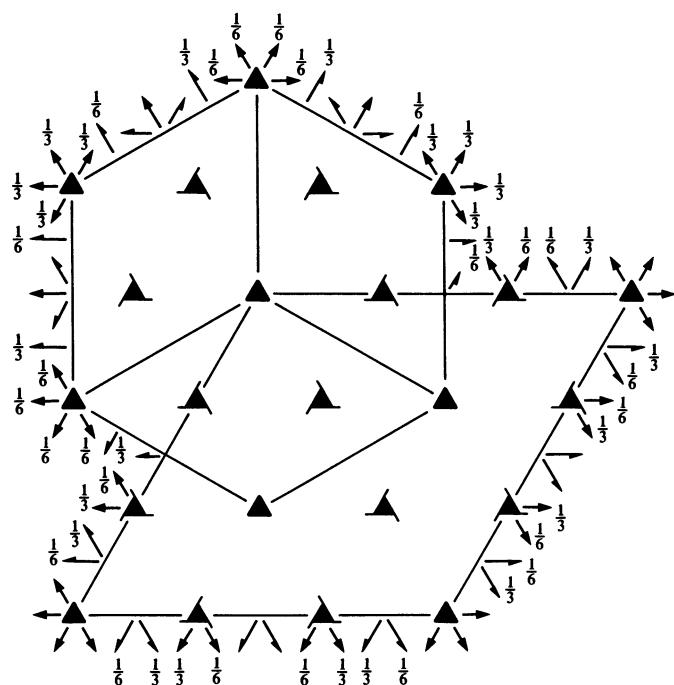
Trigonal

No. 155

$R32$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin at 32

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{6}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$
 Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{6}$ $\frac{1}{2}, 0, \frac{1}{6}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{6}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ $0, \frac{1}{2}, \frac{1}{6}$

Symmetry operations

For $(0, 0, 0)^+$ set

- | | | |
|-----------------|-------------------|-------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) 2 $x, x, 0$ | (5) 2 $x, 0, 0$ | (6) 2 $0, y, 0$ |

For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})^+$ set

- | | | |
|--|--|--|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ | (2) $3^+(0, 0, \frac{1}{3}) \frac{1}{3}, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{1}{3}) \frac{1}{3}, 0, z$ |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{6}, \frac{1}{6}$ | (5) $2(\frac{1}{2}, 0, 0) x, \frac{1}{6}, \frac{1}{6}$ | (6) 2 $\frac{1}{3}, y, \frac{1}{6}$ |

For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})^+$ set

- | | | |
|--|--|--|
| (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ | (2) $3^+(0, 0, \frac{2}{3}) 0, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{2}{3}) \frac{1}{3}, \frac{1}{3}, z$ |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{6}, \frac{1}{6}$ | (5) 2 $x, \frac{1}{3}, \frac{1}{3}$ | (6) $2(0, \frac{1}{2}, 0) \frac{1}{6}, y, \frac{1}{3}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
		$(0,0,0)+ (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+ (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$			General:
18	<i>f</i> 1	(1) x, y, z (4) y, x, \bar{z}	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, \bar{z}$	$hkil : -h + k + l = 3n$ $hki0 : -h + k = 3n$ $hh\bar{2}hl : l = 3n$ $h\bar{h}0l : h + l = 3n$ $000l : l = 3n$ $h\bar{h}00 : h = 3n$
9	<i>e</i> .2	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	Special: no extra conditions
9	<i>d</i> .2	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	
6	<i>c</i> 3.	$0, 0, z$	$0, 0, \bar{z}$		
3	<i>b</i> 32	$0, 0, \frac{1}{2}$			
3	<i>a</i> 32	$0, 0, 0$			

Symmetry of special projections

Along $[001] p3m1$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[100] p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$$

Origin at $x, 0, 0$

Along $[210] p11m$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{3}\mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	$[2] R31 (R3, 146)$	$(1; 2; 3)+$
	{ $[3] R12 (C2, 5)$	$(1; 4)+$
	{ $[3] R12 (C2, 5)$	$(1; 5)+$
	{ $[3] R12 (C2, 5)$	$(1; 6)+$
IIa	{ $[3] P3_2 21 (154)$	$1; 4; (2; 6) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3}); (3; 5) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
	{ $[3] P3_2 21 (154)$	$1; 5; (2; 4) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3}); (3; 6) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
	{ $[3] P3_2 21 (154)$	$1; 6; (2; 5) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3}); (3; 4) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
	{ $[3] P3_1 21 (152)$	$1; 4; (2; 6) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3}); (3; 5) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
	{ $[3] P3_1 21 (152)$	$1; 5; (2; 4) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3}); (3; 6) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
	{ $[3] P3_1 21 (152)$	$1; 6; (2; 5) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3}); (3; 4) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
	{ $[3] P321 (150)$	$1; 2; 3; 4; 5; 6$
	{ $[3] P321 (150)$	$1; 2; 3; (4; 5; 6) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
	{ $[3] P321 (150)$	$1; 2; 3; (4; 5; 6) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
IIIb	none	

Maximal isomorphic subgroups of lowest index

IIc $[2] R32 (\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (155)$; $[4] R32 (\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}) (155)$

Minimal non-isomorphic supergroups

I $[2] R\bar{3}m (166)$; $[2] R\bar{3}c (167)$; $[4] P432 (207)$; $[4] P4_2 32 (208)$; $[4] F432 (209)$; $[4] F4_1 32 (210)$; $[4] I432 (211)$; $[4] P4_3 32 (212)$; $[4] P4_1 32 (213)$; $[4] I4_1 32 (214)$

II $[3] P312 (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}) (149)$

$R32$

D_3^7

32

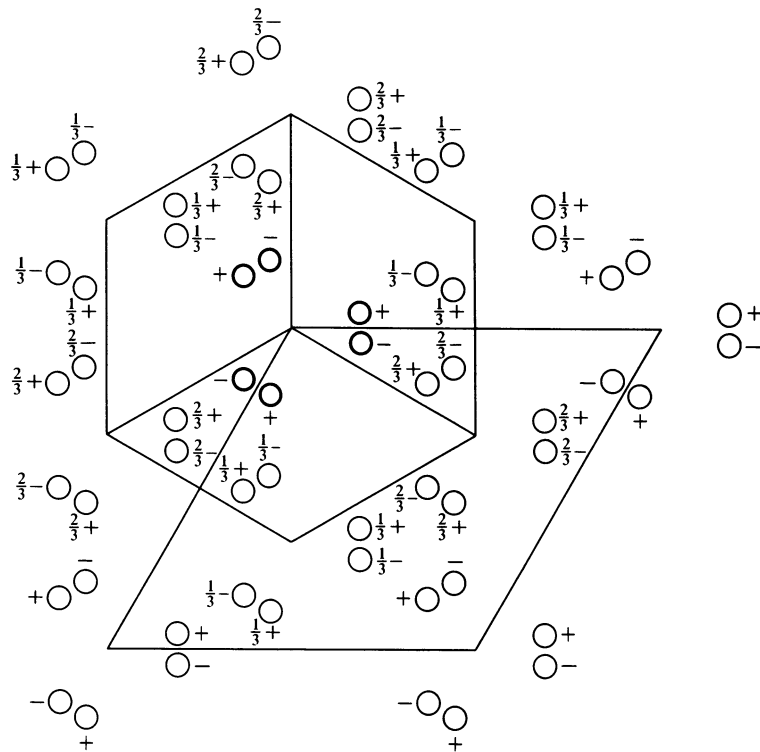
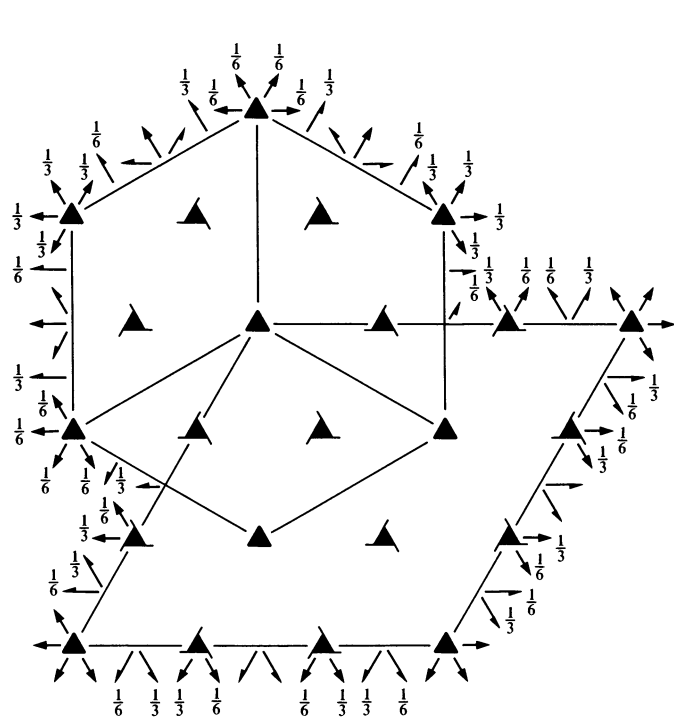
Trigonal

No. 155

$R32$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin at 32

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}; z \leq \min(x, y, 1-x, 1-y)$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1
- (2) $3^+ x, x, x$
- (3) $3^- x, x, x$
- (4) $2 \bar{x}, 0, x$
- (5) $2 x, \bar{x}, 0$
- (6) $2 0, y, \bar{y}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 <i>f</i> 1	(1) x, y, z (4) $\bar{z}, \bar{y}, \bar{x}$	(2) z, x, y (5) $\bar{y}, \bar{x}, \bar{z}$	(3) y, z, x (6) $\bar{x}, \bar{z}, \bar{y}$	General: no conditions Special: no extra conditions
3 <i>e</i> .2	$\frac{1}{2}, y, \bar{y}$	$\bar{y}, \frac{1}{2}, y$	$y, \bar{y}, \frac{1}{2}$	
3 <i>d</i> .2	$0, y, \bar{y}$	$\bar{y}, 0, y$	$y, \bar{y}, 0$	
2 <i>c</i> 3.	x, x, x	$\bar{x}, \bar{x}, \bar{x}$		
1 <i>b</i> 32	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
1 <i>a</i> 32	$0, 0, 0$			

Symmetry of special projections

Along $[111] p3m1$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[1\bar{1}0] p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, \bar{x}, 0$

Along $[2\bar{1}\bar{1}] p11m$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$$

Origin at $2x, \bar{x}, \bar{x}$

Maximal non-isomorphic subgroups

I [2] $R31 (R3, 146)$ 1; 2; 3

{ [3] $R12 (C2, 5)$ 1; 4
[3] $R12 (C2, 5)$ 1; 5
[3] $R12 (C2, 5)$ 1; 6

IIa none

IIIb [3] $P321 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}) (150)$; [3] $P3_121 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}) (152)$;

[3] $P3_221 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}) (154)$

Maximal isomorphic subgroups of lowest index

IIc [2] $R32 (\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b}) (155)$; [4] $R32 (\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}) (155)$

Minimal non-isomorphic supergroups

I [2] $R\bar{3}m (166)$; [2] $R\bar{3}c (167)$; [4] $P432 (207)$; [4] $P4_232 (208)$; [4] $F432 (209)$; [4] $F4_132 (210)$; [4] $I432 (211)$;

[4] $P4_332 (212)$; [4] $P4_132 (213)$; [4] $I4_132 (214)$

II [3] $P312 (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})) (149)$

$P3m1$

C_{3v}^1

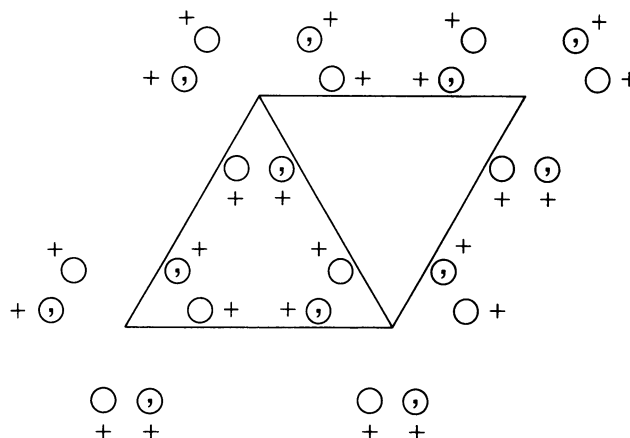
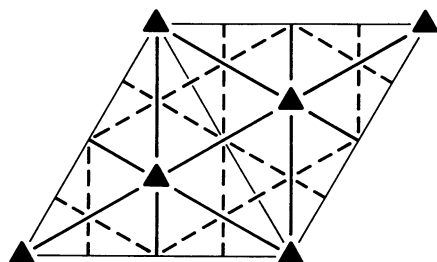
$3m1$

Trigonal

No. 156

$P3m1$

Patterson symmetry $P\bar{3}m1$



Origin on $3m1$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq 1; x \leq 2y; y \leq \min(1-x, 2x)$

Vertices $0, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
 $0, 0, 1$ $\frac{2}{3}, \frac{1}{3}, 1$ $\frac{1}{3}, \frac{2}{3}, 1$

Symmetry operations

- | | | |
|-----------------------|-------------------|-------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $m x, \bar{x}, z$ | (5) $m x, 2x, z$ | (6) $m 2x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
6 e 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) \bar{y}, \bar{x}, z (5) $\bar{x} + y, y, z$ (6) $x, x - y, z$	General: no conditions Special: no extra conditions
3 d . m .	x, \bar{x}, z $x, 2x, z$ $2\bar{x}, \bar{x}, z$	
1 c 3 m .	$\frac{2}{3}, \frac{1}{3}, z$	
1 b 3 m .	$\frac{1}{3}, \frac{2}{3}, z$	
1 a 3 m .	$0, 0, z$	

Symmetry of special projections

Along [001] $p3m1$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [100] $p1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [210] $p1m1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
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Maximal non-isomorphic subgroups

I	[2] $P311$ ($P3, 143$)	1; 2; 3
	{ [3] $P1m1$ ($Cm, 8$)	1; 4
	{ [3] $P1m1$ ($Cm, 8$)	1; 5
	{ [3] $P1m1$ ($Cm, 8$)	1; 6

IIa none

IIb [2] $P3c1$ ($\mathbf{c}' = 2\mathbf{c}$) (158); [3] $H3m1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P31m, 157$)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3m1$ ($\mathbf{c}' = 2\mathbf{c}$) (156); [4] $P3m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (156)

Minimal non-isomorphic supergroups

I	[2] $P\bar{3}m1$ (164); [2] $P6mm$ (183); [2] $P6_3mc$ (186); [2] $P\bar{6}m2$ (187)
II	[3] $H3m1$ ($P31m, 157$); [3] $R3m$ (obverse) (160); [3] $R3m$ (reverse) (160)

$P31m$

C_{3v}^2

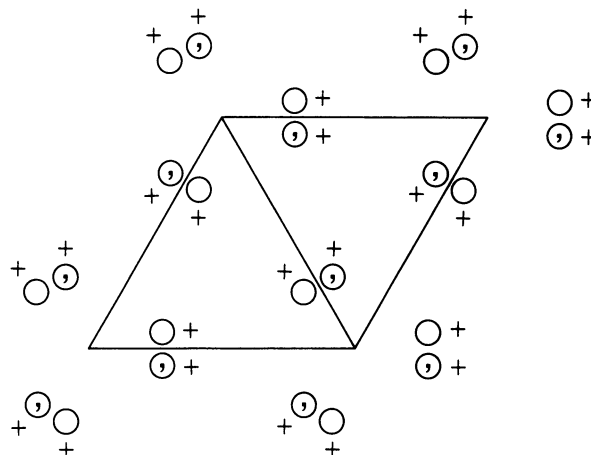
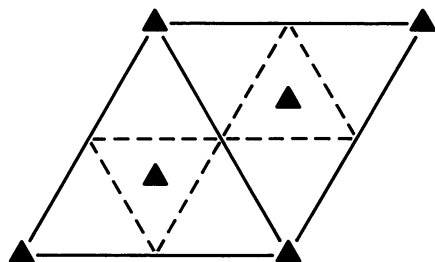
$31m$

Trigonal

No. 157

$P31m$

Patterson symmetry $P\bar{3}1m$



Origin on $31m$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{3}; 0 \leq z \leq 1; x \leq (y+1)/2; y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, 1$ $\frac{1}{2}, 0, 1$ $\frac{2}{3}, \frac{1}{3}, 1$ $\frac{1}{2}, \frac{1}{2}, 1$

Symmetry operations

- (1) 1 (2) $3^+ 0, 0, z$ (3) $3^- 0, 0, z$
 (4) $m x, x, z$ (5) $m x, 0, z$ (6) $m 0, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions	
6	d	1	(1) x, y, z (4) y, x, z	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, z$	General: no conditions Special: no extra conditions
3	c	$. . m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	
2	b	$3 . .$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$		
1	a	$3 . m$	$0, 0, z$			

Symmetry of special projections

Along $[001]$ $p31m$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[210]$ $p1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I $[2] P311 (P3, 143)$ 1; 2; 3
 { $[3] P11m (Cm, 8)$ 1; 4
 $[3] P11m (Cm, 8)$ 1; 5
 $[3] P11m (Cm, 8)$ 1; 6

IIa none

IIb $[2] P31c (\mathbf{c}' = 2\mathbf{c}) (159)$; $[3] H31m (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (P3m1, 156)$; $[3] R3m (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (160)$;
 $[3] R3m (\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (160)$

Maximal isomorphic subgroups of lowest index

IIc $[2] P31m (\mathbf{c}' = 2\mathbf{c}) (157)$; $[4] P31m (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}) (157)$

Minimal non-isomorphic supergroups

I $[2] P\bar{3}1m (162)$; $[2] P6mm (183)$; $[2] P6_3cm (185)$; $[2] P\bar{6}2m (189)$

II $[3] H31m (P3m1, 156)$

$P3c1$

C_{3v}^3

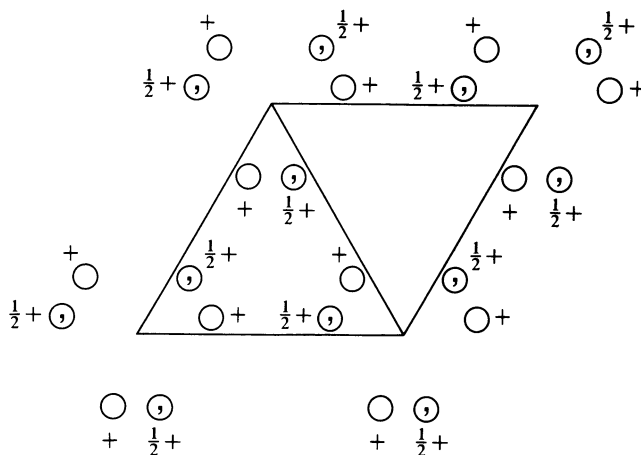
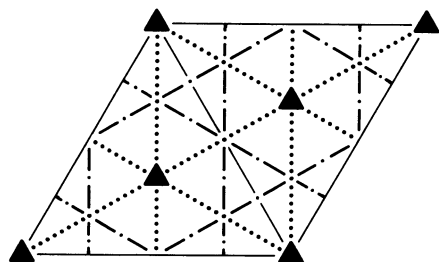
$3m1$

Trigonal

No. 158

$P3c1$

Patterson symmetry $P\bar{3}m1$



Origin on $3c1$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1
- (2) $3^+ 0, 0, z$
- (3) $3^- 0, 0, z$
- (4) $c x, \bar{x}, z$
- (5) $c x, 2x, z$
- (6) $c 2x, x, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6	<i>d</i> 1	(1) x, y, z (4) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $\bar{x} + y, y, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x, x - y, z + \frac{1}{2}$	$h\bar{h}0l : l = 2n$ $000l : l = 2n$
2	<i>c</i> 3..	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$		Special: as above, plus $hkil : l = 2n$
2	<i>b</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$		$hkil : l = 2n$
2	<i>a</i> 3..	$0, 0, z$	$0, 0, z + \frac{1}{2}$		$hkil : l = 2n$

Symmetry of special projections

Along [001] $p3m1$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p1g1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3, 143$) 1; 2; 3
 { [3] $P1c1$ ($Cc, 9$) 1; 4
 [3] $P1c1$ ($Cc, 9$) 1; 5
 [3] $P1c1$ ($Cc, 9$) 1; 6

IIa none

IIb [3] $H3c1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P31c, 159$)

Maximal isomorphic subgroups of lowest index

IIc [3] $P3c1$ ($\mathbf{c}' = 3\mathbf{c}$) (158); [4] $P3c1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (158)

Minimal non-isomorphic supergroups

I [2] $P\bar{3}c1$ (165); [2] $P6cc$ (184); [2] $P6_3cm$ (185); [2] $P\bar{6}c2$ (188)

II [3] $H3c1$ ($P31c, 159$); [3] $R3c$ (obverse) (161); [3] $R3c$ (reverse) (161); [2] $P3m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (156)

$P31c$

C_{3v}^4

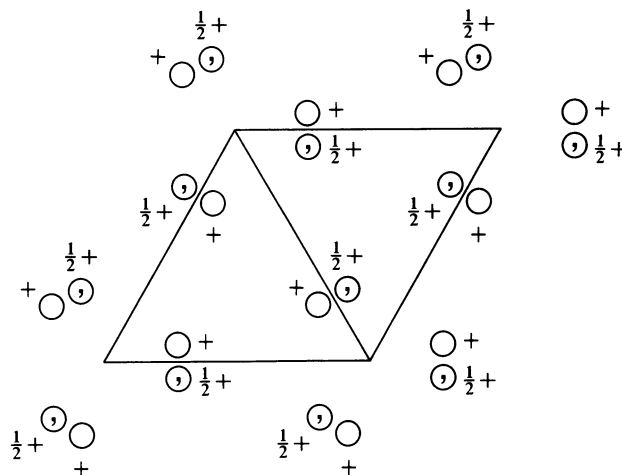
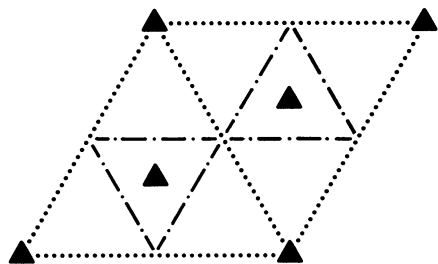
$31m$

Trigonal

No. 159

$P31c$

Patterson symmetry $P\bar{3}1m$



Origin on $31c$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1 (2) $3^+ 0, 0, z$ (3) $3^- 0, 0, z$
 (4) $c x, x, z$ (5) $c x, 0, z$ (6) $c 0, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 c 1	(1) x, y, z (4) $y, x, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$: $l = 2n$ $000l$: $l = 2n$ Special: as above, plus $hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$ $hkil$: $l = 2n$
2 b 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$		
2 a 3..	$0, 0, z$	$0, 0, z + \frac{1}{2}$		

Symmetry of special projections

Along [001] $p31m$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$	Along [100] $p1g1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along [210] $p1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
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Maximal non-isomorphic subgroups

I [2] $P311$ ($P3, 143$) 1; 2; 3
 { [3] $P11c$ ($Cc, 9$) 1; 4
 [3] $P11c$ ($Cc, 9$) 1; 5
 [3] $P11c$ ($Cc, 9$) 1; 6

IIa none

IIb [3] $H31c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3c1, 158$); [3] $R3c$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (161);
 [3] $R3c$ ($\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (161)

Maximal isomorphic subgroups of lowest index

IIc [3] $P31c$ ($\mathbf{c}' = 3\mathbf{c}$) (159); [4] $P31c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (159)

Minimal non-isomorphic supergroups

I [2] $P\bar{3}1c$ (163); [2] $P6cc$ (184); [2] $P6_3mc$ (186); [2] $P\bar{6}2c$ (190)
II [3] $H31c$ ($P3c1, 158$); [2] $P31m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (157)

$R3m$

C_{3v}^5

$3m$

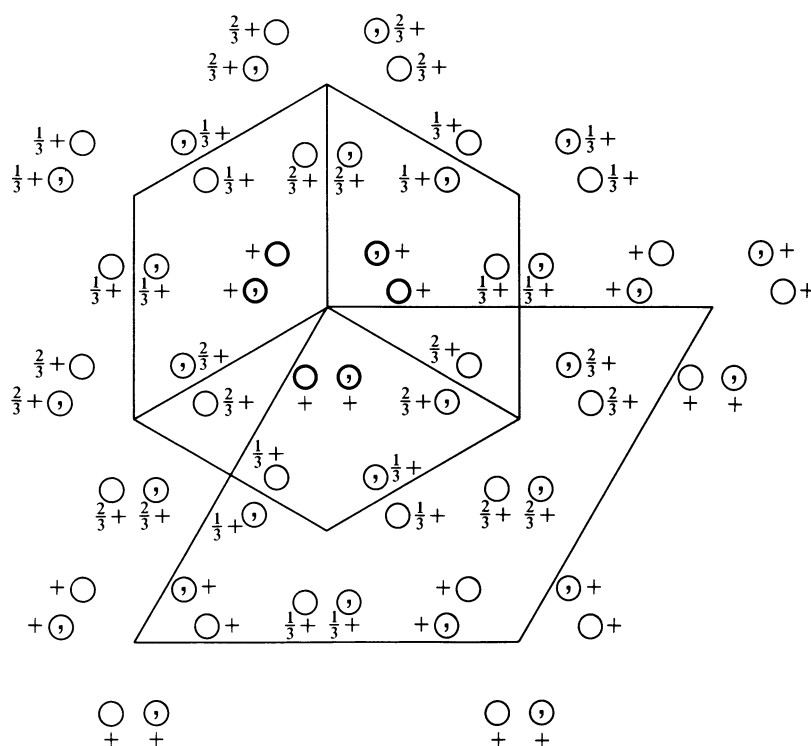
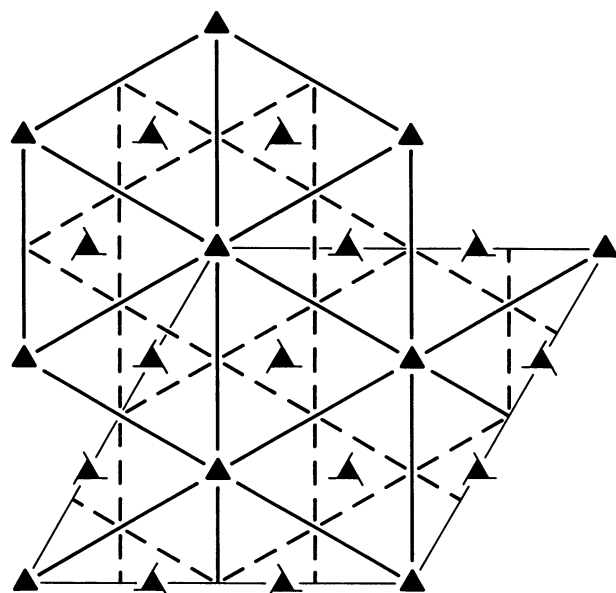
Trigonal

No. 160

$R3m$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin on $3m$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{3}; x \leq 2y; y \leq \min(1-x, 2x)$

Vertices $0, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
 $0, 0, \frac{1}{3}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$

Symmetry operations

For $(0, 0, 0)+$ set

- | | | |
|-----------------------|-------------------|-------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $m x, \bar{x}, z$ | (5) $m x, 2x, z$ | (6) $m 2x, x, z$ |

For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+$ set

- | | | |
|---|---|---|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ | (2) $3^+(0, 0, \frac{1}{3}) \frac{1}{3}, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{1}{3}) \frac{1}{3}, 0, z$ |
| (4) $g(\frac{1}{6}, -\frac{1}{6}, \frac{1}{3}) x + \frac{1}{2}, \bar{x}, z$ | (5) $g(\frac{1}{6}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{4}, 2x, z$ | (6) $g(\frac{2}{3}, \frac{1}{3}, \frac{1}{3}) 2x, x, z$ |

For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$ set

- | | | |
|---|---|---|
| (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ | (2) $3^+(0, 0, \frac{2}{3}) 0, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{2}{3}) \frac{1}{3}, \frac{1}{3}, z$ |
| (4) $g(-\frac{1}{6}, \frac{1}{6}, \frac{2}{3}) x + \frac{1}{2}, \bar{x}, z$ | (5) $g(\frac{1}{3}, \frac{2}{3}, \frac{2}{3}) x, 2x, z$ | (6) $g(\frac{1}{3}, \frac{1}{6}, \frac{2}{3}) 2x - \frac{1}{2}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2); (4)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$$(0,0,0)+ \quad (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+ \quad (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$$

18 c 1 (1) x, y, z (2) $\bar{y}, x-y, z$ (3) $\bar{x}+y, \bar{x}, z$
(4) \bar{y}, \bar{x}, z (5) $\bar{x}+y, y, z$ (6) $x, x-y, z$

Reflection conditions

General:

$$hkil : -h+k+l=3n$$

$$hki0 : -h+k=3n$$

$$hh\bar{2}hl : l=3n$$

$$h\bar{h}0l : h+l=3n$$

$$000l : l=3n$$

$$h\bar{h}00 : h=3n$$

Special: no extra conditions

9 b . m x, \bar{x}, z $x, 2x, z$ $2\bar{x}, \bar{x}, z$

3 a $3m$ $0, 0, z$

Symmetry of special projectionsAlong $[001]$ $p31m$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$ Along $[100]$ $p1$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$$

Origin at $x, 0, 0$ Along $[210]$ $p1m1$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{3}\mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$ **Maximal non-isomorphic subgroups**

I $[2] R31 (R3, 146)$ (1; 2; 3)+
 $\left\{ \begin{array}{l} [3] R1m (Cm, 8) \quad (1; 4)+ \\ [3] R1m (Cm, 8) \quad (1; 5)+ \\ [3] R1m (Cm, 8) \quad (1; 6)+ \end{array} \right.$

IIa $[3] P3m1 (156)$ 1; 2; 3; 4; 5; 6

IIIb $[2] R3c (\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (161)$

Maximal isomorphic subgroups of lowest index

IIc $[2] R3m (\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (160)$; $[4] R3m (\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}) (160)$

Minimal non-isomorphic supergroups

I $[2] R\bar{3}m (166)$; $[4] P\bar{4}3m (215)$; $[4] F\bar{4}3m (216)$; $[4] I\bar{4}3m (217)$

II $[3] P31m (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}) (157)$

$R\bar{3}m$

C_{3v}^5

$3m$

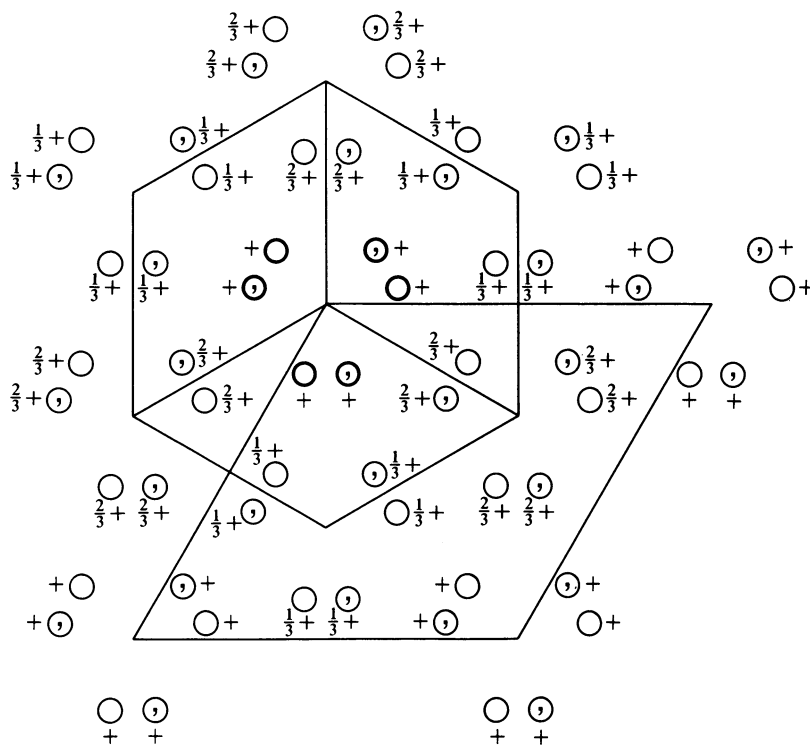
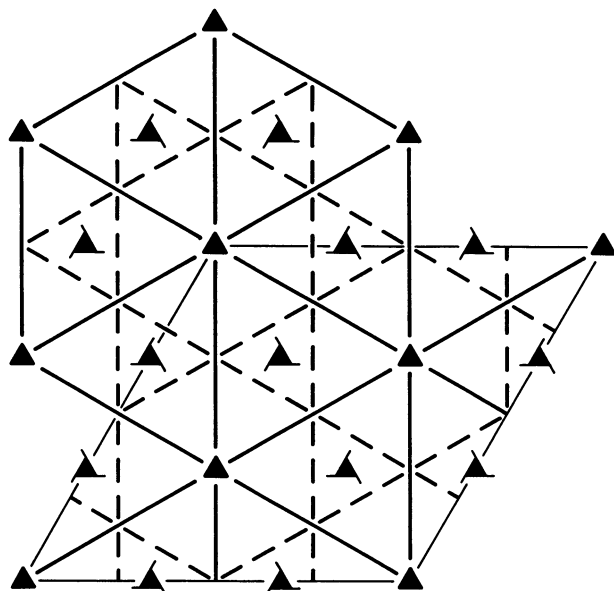
Trigonal

No. 160

$R\bar{3}m$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin on $3m$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1; y \leq x; z \leq y$

Vertices $0,0,0 \ 1,0,0 \ 1,1,0 \ 1,1,1$

Symmetry operations

- (1) 1 (2) $3^+ \ x,x,x$ (3) $3^- \ x,x,x$
 (4) $m \ x,y,x$ (5) $m \ x,x,z$ (6) $m \ x,y,y$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 c 1	(1) x,y,z (4) z,y,x	(2) z,x,y (5) y,x,z	(3) y,z,x (6) x,z,y	no conditions
3 b . m	x,x,z	z,x,x	x,z,x	Special: no extra conditions
1 a 3 m	x,x,x			

Symmetry of special projections

Along $[111] p31m$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x,x,x

Along $[1\bar{1}0] p1$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}] p1m1$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$$

Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I $\left\{ \begin{array}{ll} [2] R31 (R3, 146) & 1; 2; 3 \\ [3] R1m (Cm, 8) & 1; 4 \\ [3] R1m (Cm, 8) & 1; 5 \\ [3] R1m (Cm, 8) & 1; 6 \end{array} \right.$

IIa none

IIb $[2] F3c (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) (R3c, 161)$; $[3] P3m1 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}) (156)$

Maximal isomorphic subgroups of lowest index

IIc $[2] R3m (\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b}) (160)$; $[4] R3m (\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}) (160)$

Minimal non-isomorphic supergroups

I $[2] R\bar{3}m (166)$; $[4] P\bar{4}3m (215)$; $[4] F\bar{4}3m (216)$; $[4] I\bar{4}3m (217)$

II $[3] P31m (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})) (157)$

$R3c$

C_{3v}^6

$3m$

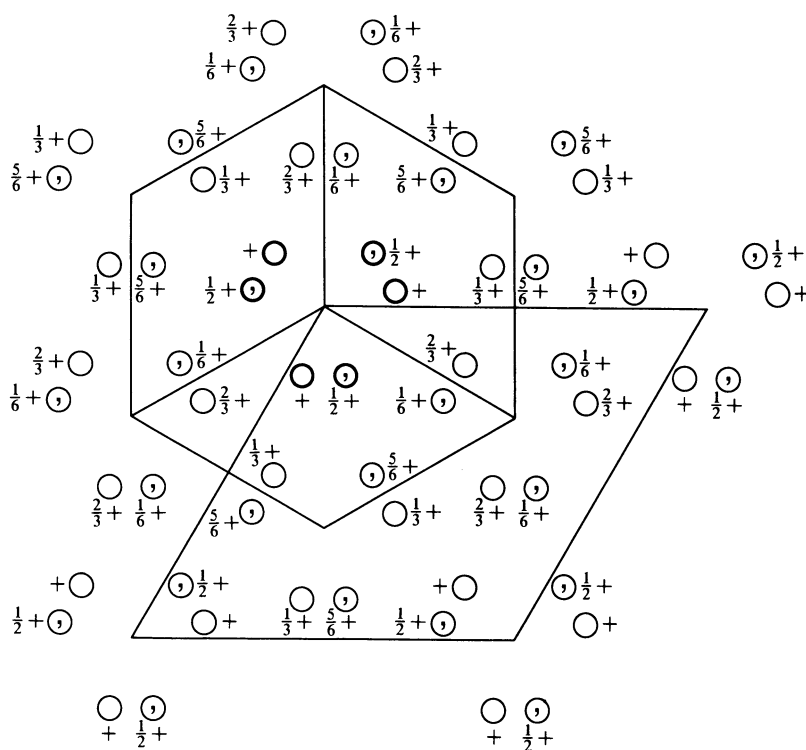
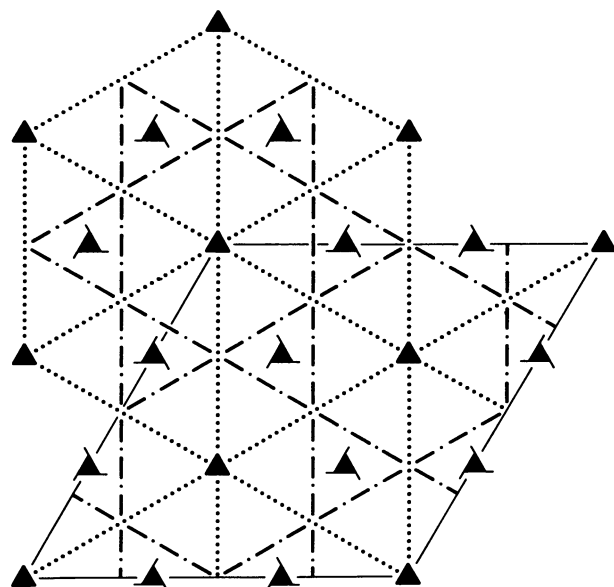
Trigonal

No. 161

$R3c$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin on $3c$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{6}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$
Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{6}$ $\frac{1}{2}, 0, \frac{1}{6}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{6}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ $0, \frac{1}{2}, \frac{1}{6}$

Symmetry operations

For $(0, 0, 0)+$ set

- | | | |
|-----------------------|-------------------|-------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $c x, \bar{x}, z$ | (5) $c x, 2x, z$ | (6) $c 2x, x, z$ |

For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+$ set

- | | | |
|---|---|---|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ | (2) $3^+(0, 0, \frac{1}{3}) \frac{1}{3}, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{1}{3}) \frac{1}{3}, 0, z$ |
| (4) $g(\frac{1}{6}, -\frac{1}{6}, \frac{5}{6}) x + \frac{1}{2}, \bar{x}, z$ | (5) $g(\frac{1}{6}, \frac{1}{3}, \frac{5}{6}) x + \frac{1}{4}, 2x, z$ | (6) $g(\frac{2}{3}, \frac{1}{3}, \frac{5}{6}) 2x, x, z$ |

For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$ set

- | | | |
|---|---|---|
| (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ | (2) $3^+(0, 0, \frac{2}{3}) 0, \frac{1}{3}, z$ | (3) $3^-(0, 0, \frac{2}{3}) \frac{1}{3}, \frac{1}{3}, z$ |
| (4) $g(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}) x + \frac{1}{2}, \bar{x}, z$ | (5) $g(\frac{1}{3}, \frac{2}{3}, \frac{1}{6}) x, 2x, z$ | (6) $g(\frac{1}{3}, \frac{1}{6}, \frac{1}{6}) 2x - \frac{1}{2}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2); (4)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$$(0,0,0)+ \left(\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right)+ \left(\frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right)+$$

18 *b* 1 (1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$
(4) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (5) $\bar{x} + y, y, z + \frac{1}{2}$ (6) $x, x - y, z + \frac{1}{2}$

Reflection conditions

General:

$$\begin{aligned} hki\bar{l} &: -h + k + l = 3n \\ hki0 &: -h + k = 3n \\ hh\bar{2}hl &: l = 3n \\ h\bar{h}0l &: h + l = 3n, \quad l = 2n \\ 000l &: l = 6n \\ h\bar{h}00 &: h = 3n \end{aligned}$$

Special: as above, plus

$$hkil : l = 2n$$

6 *a* 3. 0,0, z 0,0, $z + \frac{1}{2}$

Symmetry of special projectionsAlong [001] $p31m$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$$

Origin at 0,0, z Along [100] $p1$

$$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} + 4\mathbf{b} + \mathbf{c}) \quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$$

Origin at $x, 0, 0$ Along [210] $p1g1$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{3}\mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$ **Maximal non-isomorphic subgroups**

I [2] $R31 (R3, 146)$ (1; 2; 3)+

$$\begin{cases} [3] R1c (Cc, 9) & (1; 4)+ \\ [3] R1c (Cc, 9) & (1; 5)+ \\ [3] R1c (Cc, 9) & (1; 6)+ \end{cases}$$

IIa [3] $P3c1 (158)$ 1; 2; 3; 4; 5; 6

IIb none

Maximal isomorphic subgroups of lowest index

IIc [4] $R3c (\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}) (161)$; [5] $R3c (\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 5\mathbf{c}) (161)$

Minimal non-isomorphic supergroups

I [2] $R\bar{3}c (167)$; [4] $P\bar{4}3n (218)$; [4] $F\bar{4}3c (219)$; [4] $I\bar{4}3d (220)$

II [2] $R3m (\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (160)$; [3] $P31c (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}) (159)$

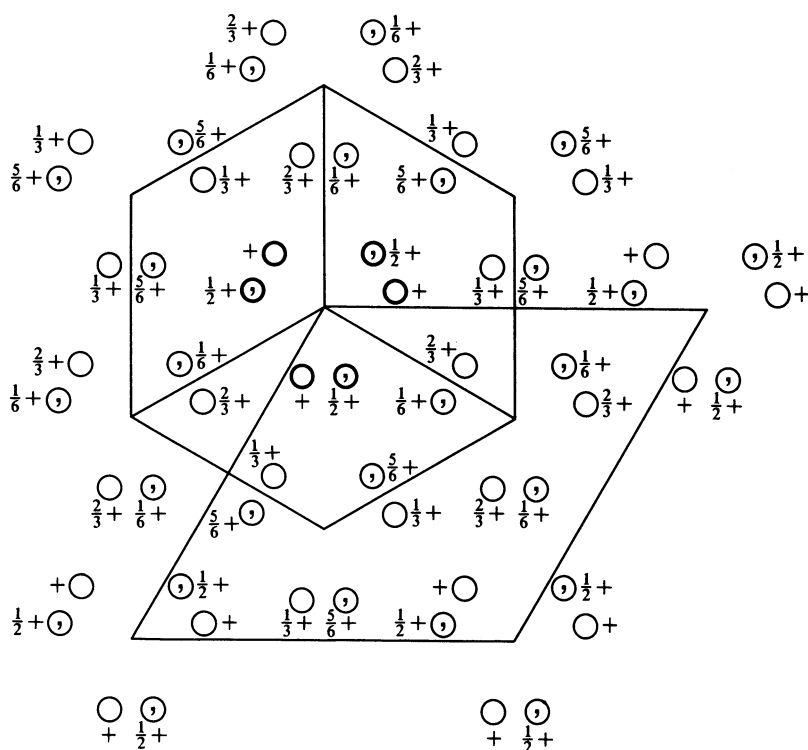
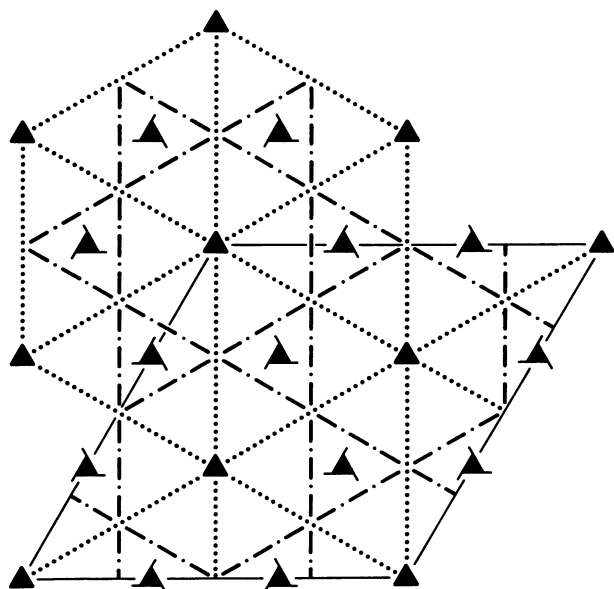
$R\bar{3}c$ C_{3v}^6 $3m$

Trigonal

No. 161

 $R\bar{3}c$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES

**Origin** on $3c$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1; y \leq x; z \leq y$
 Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 1,1,1$

Symmetry operations

- (1) 1 (2) $3^+ x, x, x$ (3) $3^- x, x, x$
 (4) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, x$ (5) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, z$ (6) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, y$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 <i>b</i> 1	(1) x, y, z (4) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	(2) z, x, y (5) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(3) y, z, x (6) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	$hhl : l = 2n$ $hhh : h = 2n$
2 <i>a</i> 3.	x, x, x	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$		Special: as above, plus $hkl : h + k + l = 2n$

Symmetry of special projections

Along $[111] p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along $[1\bar{1}0] p1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, \bar{x}, 0$	Along $[2\bar{1}\bar{1}] p1g1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ Origin at $2x, \bar{x}, \bar{x}$
---	---	--

Maximal non-isomorphic subgroups

I	[2] $R31 (R3, 146)$	1; 2; 3	
	{	[3] $R1c (Cc, 9)$	1; 4
		[3] $R1c (Cc, 9)$	1; 5
		[3] $R1c (Cc, 9)$	1; 6

IIa none

IIIb [3] $P3c1 (\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}) (158)$

Maximal isomorphic subgroups of lowest index

IIc [4] $R3c (\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}) (161)$; [5] $R3c (\mathbf{a}' = \mathbf{a} + 2\mathbf{b} + 2\mathbf{c}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b} + 2\mathbf{c}, \mathbf{c}' = 2\mathbf{a} + 2\mathbf{b} + \mathbf{c}) (161)$

Minimal non-isomorphic supergroups

I	[2] $R\bar{3}c (167)$; [4] $P\bar{4}3n (218)$; [4] $F\bar{4}3c (219)$; [4] $I\bar{4}3d (220)$
II	[2] $R3m (\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}), \mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}), \mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})) (160)$; [3] $P31c (\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})) (159)$

$P\bar{3}1m$

D_{3d}^1

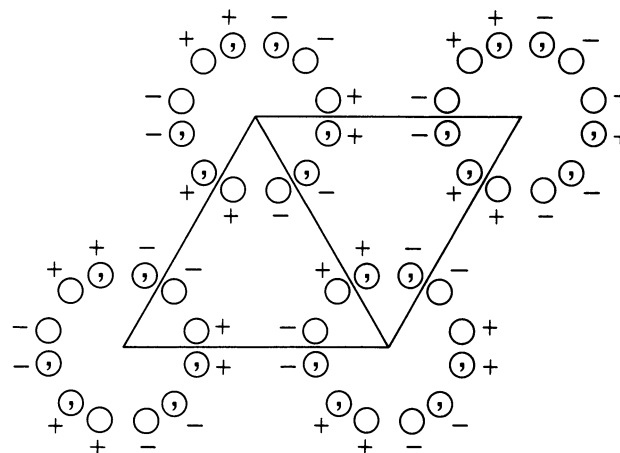
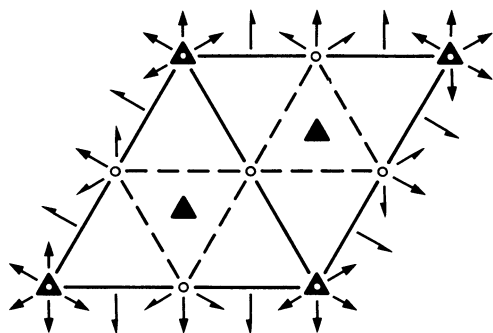
$\bar{3}1m$

Trigonal

No. 162

$P\bar{3}12/m$

Patterson symmetry $P\bar{3}1m$



Origin at centre ($\bar{3}1m$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|-----------------------|----------------------------------|----------------------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) 2 $x, \bar{x}, 0$ | (5) 2 $x, 2x, 0$ | (6) 2 $2x, x, 0$ |
| (7) $\bar{1} 0, 0, 0$ | (8) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (9) $\bar{3}^- 0, 0, z; 0, 0, 0$ |
| (10) $m x, x, z$ | (11) $m x, 0, z$ | (12) $m 0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>l</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $\bar{y}, \bar{x}, \bar{z}$ (5) $\bar{x} + y, y, \bar{z}$ (6) $x, x - y, \bar{z}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (9) $x - y, x, \bar{z}$ (10) y, x, z (11) $x - y, \bar{y}, z$ (12) $\bar{x}, \bar{x} + y, z$	General: no conditions Special: no extra conditions
6 <i>k</i> .. <i>m</i>	$x, 0, z$ $0, x, z$ \bar{x}, \bar{x}, z $0, \bar{x}, \bar{z}$ $\bar{x}, 0, \bar{z}$ x, x, \bar{z}	
6 <i>j</i> .. 2	$x, \bar{x}, \frac{1}{2}$ $x, 2x, \frac{1}{2}$ $2\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$ $\bar{x}, 2\bar{x}, \frac{1}{2}$ $2x, x, \frac{1}{2}$	
6 <i>i</i> .. 2	$x, \bar{x}, 0$ $x, 2x, 0$ $2\bar{x}, \bar{x}, 0$ $\bar{x}, x, 0$ $\bar{x}, 2\bar{x}, 0$ $2x, x, 0$	
4 <i>h</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{1}{3}, \frac{2}{3}, \bar{z}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$ $\frac{2}{3}, \frac{1}{3}, z$	
3 <i>g</i> .. $2/m$	$\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
3 <i>f</i> .. $2/m$	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	
2 <i>e</i> 3. <i>m</i>	$0, 0, z$ $0, 0, \bar{z}$	
2 <i>d</i> 3. 2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$	
2 <i>c</i> 3. 2	$\frac{1}{3}, \frac{2}{3}, 0$ $\frac{2}{3}, \frac{1}{3}, 0$	
1 <i>b</i> $\bar{3}.m$	$0, 0, \frac{1}{2}$	
1 <i>a</i> $\bar{3}.m$	$0, 0, 0$	

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{3}1m$ (157)	1; 2; 3; 10; 11; 12
	[2] $P\bar{3}12$ (149)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}, 147$)	1; 2; 3; 7; 8; 9
	{ [3] $P112/m$ ($C2/m, 12$)	1; 4; 7; 10
	{ [3] $P112/m$ ($C2/m, 12$)	1; 5; 7; 11
	{ [3] $P112/m$ ($C2/m, 12$)	1; 6; 7; 12

IIa none

IIb [2] $P\bar{3}1c$ ($\mathbf{c}' = 2\mathbf{c}$) (163); [3] $H\bar{3}1m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{3}m1, 164$); [3] $R\bar{3}m$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (166); [3] $R\bar{3}m$ ($\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (166)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}1m$ ($\mathbf{c}' = 2\mathbf{c}$) (162); [4] $P\bar{3}1m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (162)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)

II [3] $H\bar{3}1m$ ($P\bar{3}m1, 164$)

$P\bar{3}1c$

D_{3d}^2

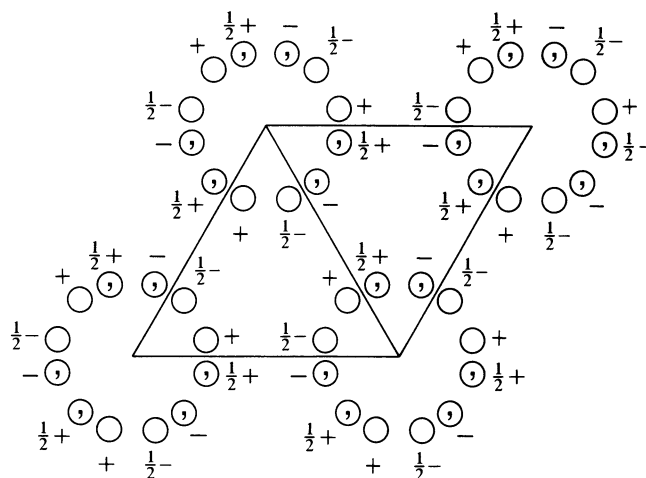
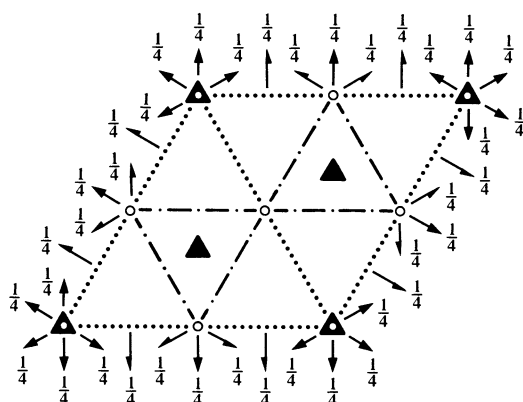
$\bar{3}1m$

Trigonal

No. 163

$P\bar{3}12/c$

Patterson symmetry $P\bar{3}1m$



Origin at centre ($\bar{3}$) at $\bar{3}1c$

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{4}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|---------------------------------|---------------------------------------|---------------------------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) 2 $x, \bar{x}, \frac{1}{4}$ | (5) 2 $x, 2x, \frac{1}{4}$ | (6) 2 $2x, x, \frac{1}{4}$ |
| (7) $\bar{1}$ $0, 0, 0$ | (8) $\bar{3}^+$ $0, 0, z$; $0, 0, 0$ | (9) $\bar{3}^-$ $0, 0, z$; $0, 0, 0$ |
| (10) c x, x, z | (11) c $x, 0, z$ | (12) c $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>i</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (5) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$ (6) $x, x - y, \bar{z} + \frac{1}{2}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (9) $x - y, x, \bar{z}$ (10) $y, x, z + \frac{1}{2}$ (11) $x - y, \bar{y}, z + \frac{1}{2}$ (12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$: $l = 2n$ $000l$: $l = 2n$
6 <i>h</i> ..2	$x, \bar{x}, \frac{1}{4}$ $x, 2x, \frac{1}{4}$ $2\bar{x}, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$ $\bar{x}, 2\bar{x}, \frac{3}{4}$ $2x, x, \frac{3}{4}$	Special: as above, plus no extra conditions
6 <i>g</i> $\bar{1}$	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil$: $l = 2n$
4 <i>f</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> 3..	$0, 0, z$ $0, 0, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, z + \frac{1}{2}$	$hkil$: $l = 2n$
2 <i>d</i> 3.2	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> 3.2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>b</i> $\bar{3}$..	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkil$: $l = 2n$
2 <i>a</i> 3.2	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkil$: $l = 2n$

Symmetry of special projections

Along $[001]$ $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[210]$ $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P312$ (149)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}$, 147)	1; 2; 3; 7; 8; 9
	{ [3] $P112/c$ ($C2/c$, 15)	1; 4; 7; 10
	{ [3] $P112/c$ ($C2/c$, 15)	1; 5; 7; 11
	{ [3] $P112/c$ ($C2/c$, 15)	1; 6; 7; 12

IIa none

IIb [3] $H\bar{3}1c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{3}c1$, 165); [3] $R\bar{3}c$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (167);
[3] $R\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (167)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{3}1c$ ($\mathbf{c}' = 3\mathbf{c}$) (163); [4] $P\bar{3}1c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (163)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

II [3] $H\bar{3}1c$ ($P\bar{3}c1$, 165); [2] $P\bar{3}1m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (162)

$P\bar{3}m1$

D_{3d}^3

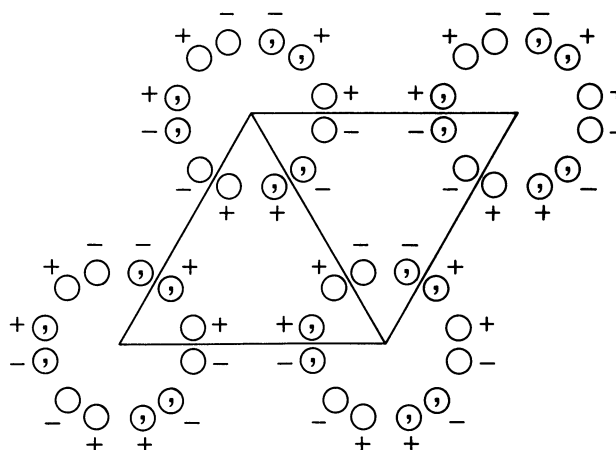
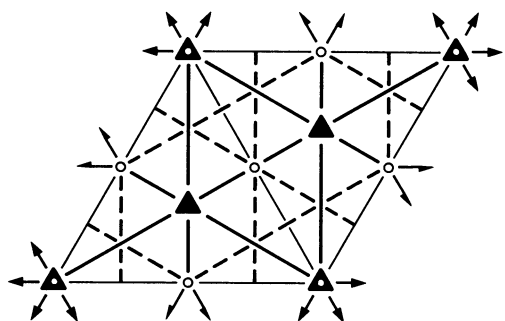
$\bar{3}m1$

Trigonal

No. 164

$P\bar{3}2/m1$

Patterson symmetry $P\bar{3}m1$



Origin at centre ($\bar{3}m1$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{3}$; $0 \leq z \leq 1$; $x \leq (1+y)/2$; $y \leq x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$
 $0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$

Symmetry operations

- | | | |
|------------------------|-----------------------------------|-----------------------------------|
| (1) 1 | (2) 3^+ $0,0,z$ | (3) 3^- $0,0,z$ |
| (4) 2 $x,x,0$ | (5) 2 $x,0,0$ | (6) 2 $0,y,0$ |
| (7) $\bar{1}$ $0,0,0$ | (8) $\bar{3}^+$ $0,0,z$; $0,0,0$ | (9) $\bar{3}^-$ $0,0,z$; $0,0,0$ |
| (10) m x,\bar{x},z | (11) m $x,2x,z$ | (12) m $2x,x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>j</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) y, x, \bar{z} (5) $x - y, \bar{y}, \bar{z}$ (6) $\bar{x}, \bar{x} + y, \bar{z}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (9) $x - y, x, \bar{z}$ (10) \bar{y}, \bar{x}, z (11) $\bar{x} + y, y, z$ (12) $x, x - y, z$	General: no conditions Special: no extra conditions
6 <i>i</i> . <i>m</i> .	x, \bar{x}, z $x, 2x, z$ $2\bar{x}, \bar{x}, z$ \bar{x}, x, \bar{z} $2x, x, \bar{z}$ $\bar{x}, 2\bar{x}, \bar{z}$	
6 <i>h</i> .2.	$x, 0, \frac{1}{2}$ $0, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $x, x, \frac{1}{2}$	
6 <i>g</i> .2.	$x, 0, 0$ $0, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, 0, 0$ $0, \bar{x}, 0$ $x, x, 0$	
3 <i>f</i> . $2/m$.	$\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
3 <i>e</i> . $2/m$.	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	
2 <i>d</i> 3 <i>m</i> .	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$	
2 <i>c</i> 3 <i>m</i> .	$0, 0, z$ $0, 0, \bar{z}$	
1 <i>b</i> $\bar{3}m$.	$0, 0, \frac{1}{2}$	
1 <i>a</i> $\bar{3}m$.	$0, 0, 0$	

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{3}m1$ (156)	1; 2; 3; 10; 11; 12
	[2] $P\bar{3}21$ (150)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}$, 147)	1; 2; 3; 7; 8; 9
	{ [3] $P12/m1$ ($C2/m$, 12)	1; 4; 7; 10
	{ [3] $P12/m1$ ($C2/m$, 12)	1; 5; 7; 11
	{ [3] $P12/m1$ ($C2/m$, 12)	1; 6; 7; 12

IIa none

IIb [2] $P\bar{3}c1$ ($\mathbf{c}' = 2\mathbf{c}$) (165); [3] $H\bar{3}m1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{3}1m$, 162)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}m1$ ($\mathbf{c}' = 2\mathbf{c}$) (164); [4] $P\bar{3}m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (164)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II [3] $H\bar{3}m1$ ($P\bar{3}1m$, 162); [3] $R\bar{3}m$ (obverse) (166); [3] $R\bar{3}m$ (reverse) (166)

$P\bar{3}c1$

D_{3d}^4

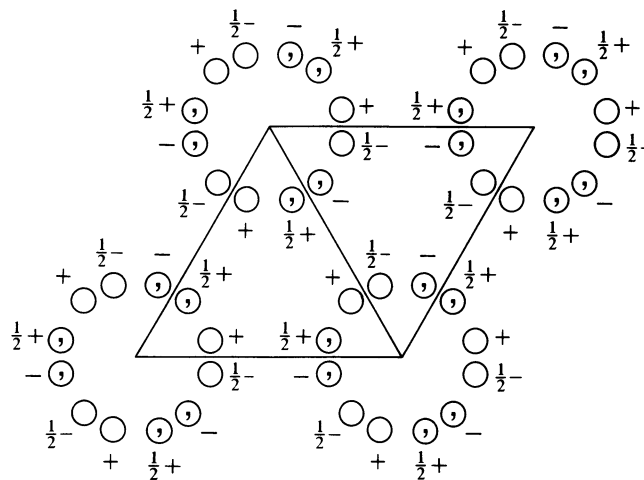
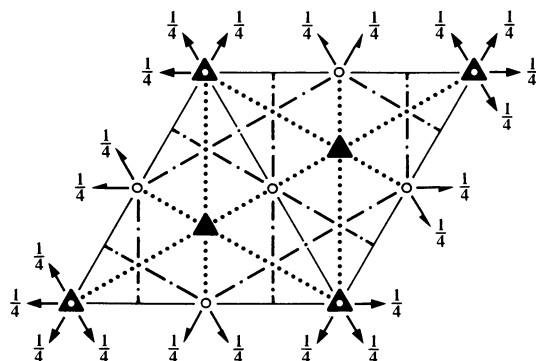
$\bar{3}m1$

Trigonal

No. 165

$P\bar{3}2/c1$

Patterson symmetry $P\bar{3}m1$



Origin at centre ($\bar{3}$) at $\bar{3}c1$

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{4}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|---------------------------|---------------------------------------|---------------------------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) 2 $x, x, \frac{1}{4}$ | (5) 2 $x, 0, \frac{1}{4}$ | (6) 2 $0, y, \frac{1}{4}$ |
| (7) $\bar{1}$ $0, 0, 0$ | (8) $\bar{3}^+$ $0, 0, z$; $0, 0, 0$ | (9) $\bar{3}^-$ $0, 0, z$; $0, 0, 0$ |
| (10) c x, \bar{x}, z | (11) c $x, 2x, z$ | (12) c $2x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates								Reflection conditions
									General:
12 <i>g</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$						$h\bar{h}0l : l = 2n$
	(4) $y, x, \bar{z} + \frac{1}{2}$	(5) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$	(6) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$						$000l : l = 2n$
	(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $y, \bar{x} + y, \bar{z}$	(9) $x - y, x, \bar{z}$						
	(10) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(11) $\bar{x} + y, y, z + \frac{1}{2}$	(12) $x, x - y, z + \frac{1}{2}$						
									Special: as above, plus
6 <i>f</i> .2.	$x, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	no extra conditions		
6 <i>e</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil : l = 2n$		
4 <i>d</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z} + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$		$hkil : l = 2n$			
4 <i>c</i> 3..	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$		$hkil : l = 2n$			
2 <i>b</i> $\bar{3}$..	$0, 0, 0$	$0, 0, \frac{1}{2}$						$hkil : l = 2n$	
2 <i>a</i> 32.	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$						$hkil : l = 2n$	

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P3c1$ (158)	1; 2; 3; 10; 11; 12
	[2] $P321$ (150)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}$, 147)	1; 2; 3; 7; 8; 9
	{ [3] $P12/c1$ ($C2/c$, 15)	1; 4; 7; 10
	{ [3] $P12/c1$ ($C2/c$, 15)	1; 5; 7; 11
	{ [3] $P12/c1$ ($C2/c$, 15)	1; 6; 7; 12

IIa none

IIb [3] $H\bar{3}c1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{3}1c$, 163)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{3}c1$ ($\mathbf{c}' = 3\mathbf{c}$) (165); [4] $P\bar{3}c1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (165)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

II [3] $H\bar{3}c1$ ($P\bar{3}1c$, 163); [3] $R\bar{3}c$ (obverse) (167); [3] $R\bar{3}c$ (reverse) (167); [2] $P\bar{3}m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (164)

$R\bar{3}m$

D_{3d}^5

$\bar{3}m$

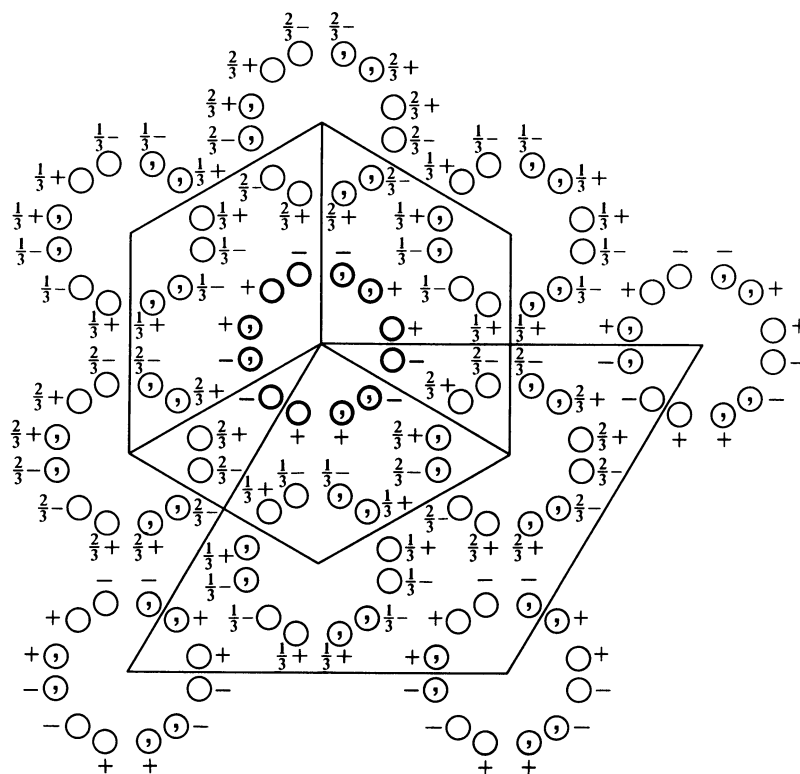
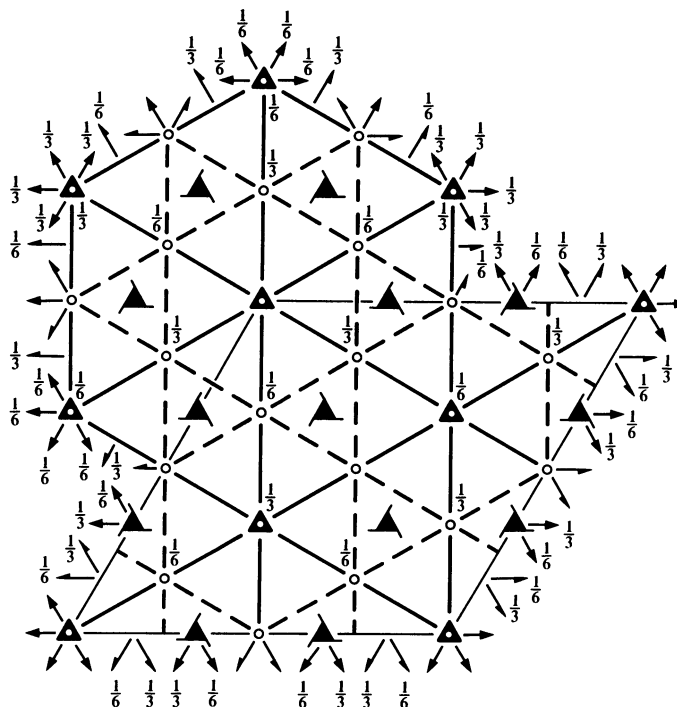
Trigonal

No. 166

$R\bar{3}2/m$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin at centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{6}$; $x \leq 2y$; $y \leq \min(1-x, 2x)$

Vertices $0, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
 $0, 0, \frac{1}{6}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{6}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{6}$

Symmetry operations

For (0,0,0)+ set

- | | | |
|----------------------|------------------------------|------------------------------|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) $2 x,x,0$ | (5) $2 x,0,0$ | (6) $2 0,y,0$ |
| (7) $\bar{1} 0,0,0$ | (8) $\bar{3}^+ 0,0,z; 0,0,0$ | (9) $\bar{3}^- 0,0,z; 0,0,0$ |
| (10) $m x,\bar{x},z$ | (11) $m x,2x,z$ | (12) $m 2x,x,z$ |

For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ + set

- | | | |
|--|--|--|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ | (2) $3^+(0,0,\frac{1}{3}) \frac{1}{3}, \frac{1}{3}, z$ | (3) $3^-(0,0,\frac{1}{3}) \frac{1}{3}, 0, z$ |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{6}, \frac{1}{6}$ | (5) $2(\frac{1}{2}, 0, 0) x, \frac{1}{6}, \frac{1}{6}$ | (6) $2 \frac{1}{3}, y, \frac{1}{6}$ |
| (7) $\bar{1} \frac{1}{3}, \frac{1}{6}, \frac{1}{6}$ | (8) $\bar{3}^+ \frac{1}{3}, -\frac{1}{3}, z; \frac{1}{3}, -\frac{1}{3}, \frac{1}{6}$ | (9) $\bar{3}^- \frac{1}{3}, \frac{2}{3}, z; \frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ |
| (10) $g(\frac{1}{6}, -\frac{1}{6}, \frac{1}{3}) x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{6}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{4}, 2x, z$ | (12) $g(\frac{2}{3}, \frac{1}{3}, \frac{1}{3}) 2x, x, z$ |

For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ + set

- | | | |
|--|--|--|
| (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ | (2) $3^+(0,0,\frac{2}{3}) 0, \frac{1}{3}, z$ | (3) $3^-(0,0,\frac{2}{3}) \frac{1}{3}, \frac{1}{3}, z$ |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{6}, \frac{1}{3}$ | (5) $2 x, \frac{1}{3}, \frac{1}{3}$ | (6) $2(0, \frac{1}{2}, 0) \frac{1}{6}, y, \frac{1}{3}$ |
| (7) $\bar{1} \frac{1}{6}, \frac{1}{3}, \frac{1}{3}$ | (8) $\bar{3}^+ \frac{2}{3}, \frac{1}{3}, z; \frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ | (9) $\bar{3}^- -\frac{1}{3}, \frac{1}{3}, z; -\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ |
| (10) $g(-\frac{1}{6}, \frac{1}{6}, \frac{2}{3}) x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{3}, \frac{2}{3}, \frac{2}{3}) x, 2x, z$ | (12) $g(\frac{1}{3}, \frac{1}{6}, \frac{2}{3}) 2x - \frac{1}{2}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

(0,0,0)+ $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ +

Reflection conditions

General:

- | | | | | | |
|----|----------|---|---------------------------------|-------------------------------|-------------------------------------|
| 36 | <i>i</i> | 1 | (1) x, y, z | (2) $\bar{y}, x - y, z$ | (3) $\bar{x} + y, \bar{x}, z$ |
| | | | (4) y, x, \bar{z} | (5) $x - y, \bar{y}, \bar{z}$ | (6) $\bar{x}, \bar{x} + y, \bar{z}$ |
| | | | (7) $\bar{x}, \bar{y}, \bar{z}$ | (8) $y, \bar{x} + y, \bar{z}$ | (9) $x - y, x, \bar{z}$ |
| | | | (10) \bar{y}, \bar{x}, z | (11) $\bar{x} + y, y, z$ | (12) $x, x - y, z$ |

- $hkil : -h + k + l = 3n$
 $hki0 : -h + k = 3n$
 $hh\bar{2}hl : l = 3n$
 $h\bar{h}0l : h + l = 3n$
 $000l : l = 3n$
 $h\bar{h}00 : h = 3n$

Special: no extra conditions

- | | | | | | | | | |
|----|----------|--------------|-------------------------------|-------------------------------|---|---------------------------|---------------------------|------------------------------|
| 18 | <i>h</i> | . <i>m</i> | x, \bar{x}, z | $x, 2x, z$ | $2\bar{x}, \bar{x}, z$ | \bar{x}, x, \bar{z} | $2x, x, \bar{z}$ | $\bar{x}, 2\bar{x}, \bar{z}$ |
| 18 | <i>g</i> | . <i>2</i> | $x, 0, \frac{1}{2}$ | $0, x, \frac{1}{2}$ | $\bar{x}, \bar{x}, \frac{1}{2}$ | $\bar{x}, 0, \frac{1}{2}$ | $0, \bar{x}, \frac{1}{2}$ | $x, x, \frac{1}{2}$ |
| 18 | <i>f</i> | . <i>2</i> | $x, 0, 0$ | $0, x, 0$ | $\bar{x}, \bar{x}, 0$ | $\bar{x}, 0, 0$ | $0, \bar{x}, 0$ | $x, x, 0$ |
| 9 | <i>e</i> | . <i>2/m</i> | $\frac{1}{2}, 0, 0$ | $0, \frac{1}{2}, 0$ | $\frac{1}{2}, \frac{1}{2}, 0$ | | | |
| 9 | <i>d</i> | . <i>2/m</i> | $\frac{1}{2}, 0, \frac{1}{2}$ | $0, \frac{1}{2}, \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | | | |
| 6 | <i>c</i> | <i>3m</i> | $0, 0, z$ | $0, 0, \bar{z}$ | | | | |
| 3 | <i>b</i> | $\bar{3}m$ | $0, 0, \frac{1}{2}$ | | | | | |
| 3 | <i>a</i> | $\bar{3}m$ | $0, 0, 0$ | | | | | |

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$
 Origin at 0, 0, z

Along [100] $p2$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$
 Origin at x, 0, 0

Along [210] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I	[2] $R\bar{3}m$ (160)	(1; 2; 3; 10; 11; 12)+
	[2] $R\bar{3}2$ (155)	(1; 2; 3; 4; 5; 6)+
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	(1; 2; 3; 7; 8; 9)+
	{ [3] $R12/m$ ($C2/m$, 12)	(1; 4; 7; 10)+
	{ [3] $R12/m$ ($C2/m$, 12)	(1; 5; 7; 11)+
	{ [3] $R12/m$ ($C2/m$, 12)	(1; 6; 7; 12)+

IIa	{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
	{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$

IIb	[2] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (167)
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Maximal isomorphic subgroups of lowest index

IIc	[2] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (166)
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Minimal non-isomorphic supergroups

I	[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)
II	[3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (162)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I	[2] $R\bar{3}m$ (160)	1; 2; 3; 10; 11; 12
	[2] $R\bar{3}2$ (155)	1; 2; 3; 4; 5; 6
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	1; 2; 3; 7; 8; 9
	{ [3] $R12/m$ ($C2/m$, 12)	1; 4; 7; 10
	{ [3] $R12/m$ ($C2/m$, 12)	1; 5; 7; 11
	{ [3] $R12/m$ ($C2/m$, 12)	1; 6; 7; 12

IIa	none
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IIb	[2] $F\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($R\bar{3}c$, 167); [3] $P\bar{3}m1$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$) (164)
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Maximal isomorphic subgroups of lowest index

IIc	[2] $R\bar{3}m$ ($\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}$) (166)
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Minimal non-isomorphic supergroups

I	[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)
II	[3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$) (162)

Trigonal

$\bar{3}m$

D_{3d}^5

$R\bar{3}m$

Patterson symmetry $R\bar{3}m$

$R\bar{3}2/m$

No. 166

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

Origin at centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}; y \leq x; z \leq \min(y, 1-x)$
Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|-----------------------|----------------------------------|----------------------------------|
| (1) 1 | (2) $3^+ x, x, x$ | (3) $3^- x, x, x$ |
| (4) 2 $\bar{x}, 0, x$ | (5) 2 $x, \bar{x}, 0$ | (6) 2 $0, y, \bar{y}$ |
| (7) $\bar{1} 0, 0, 0$ | (8) $\bar{3}^+ x, x, x; 0, 0, 0$ | (9) $\bar{3}^- x, x, x; 0, 0, 0$ |
| (10) $m x, y, x$ | (11) $m x, x, z$ | (12) $m x, y, y$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>i</i> 1	(1) x, y, z (2) z, x, y (3) y, z, x (4) $\bar{z}, \bar{y}, \bar{x}$ (5) $\bar{y}, \bar{x}, \bar{z}$ (6) $\bar{x}, \bar{z}, \bar{y}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (8) $\bar{z}, \bar{x}, \bar{y}$ (9) $\bar{y}, \bar{z}, \bar{x}$ (10) z, y, x (11) y, x, z (12) x, z, y	General: no conditions Special: no extra conditions
6 <i>h</i> . <i>m</i>	$x, x, z \quad z, x, x \quad x, z, x \quad \bar{z}, \bar{x}, \bar{x} \quad \bar{x}, \bar{x}, \bar{z} \quad \bar{x}, \bar{z}, \bar{x}$	
6 <i>g</i> .2	$x, \bar{x}, \frac{1}{2} \quad \frac{1}{2}, x, \bar{x} \quad \bar{x}, \frac{1}{2}, x \quad \bar{x}, x, \frac{1}{2} \quad \frac{1}{2}, \bar{x}, x \quad x, \frac{1}{2}, \bar{x}$	
6 <i>f</i> .2	$x, \bar{x}, 0 \quad 0, x, \bar{x} \quad \bar{x}, 0, x \quad \bar{x}, x, 0 \quad 0, \bar{x}, x \quad x, 0, \bar{x}$	
3 <i>e</i> . $2/m$	$0, \frac{1}{2}, \frac{1}{2} \quad \frac{1}{2}, 0, \frac{1}{2} \quad \frac{1}{2}, \frac{1}{2}, 0$	
3 <i>d</i> . $2/m$	$\frac{1}{2}, 0, 0 \quad 0, \frac{1}{2}, 0 \quad 0, 0, \frac{1}{2}$	
2 <i>c</i> 3 <i>m</i>	$x, x, x \quad \bar{x}, \bar{x}, \bar{x}$	
1 <i>b</i> $\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	
1 <i>a</i> $\bar{3}m$	$0, 0, 0$	

Symmetry of special projections

Along $[111] p6mm$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along $[1\bar{1}0] p2$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \bar{x}, 0$	Along $[2\bar{1}\bar{1}] p2mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ Origin at $2x, \bar{x}, \bar{x}$
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(Continued on preceding page)

$R\bar{3}c$

D_{3d}^6

$\bar{3}m$

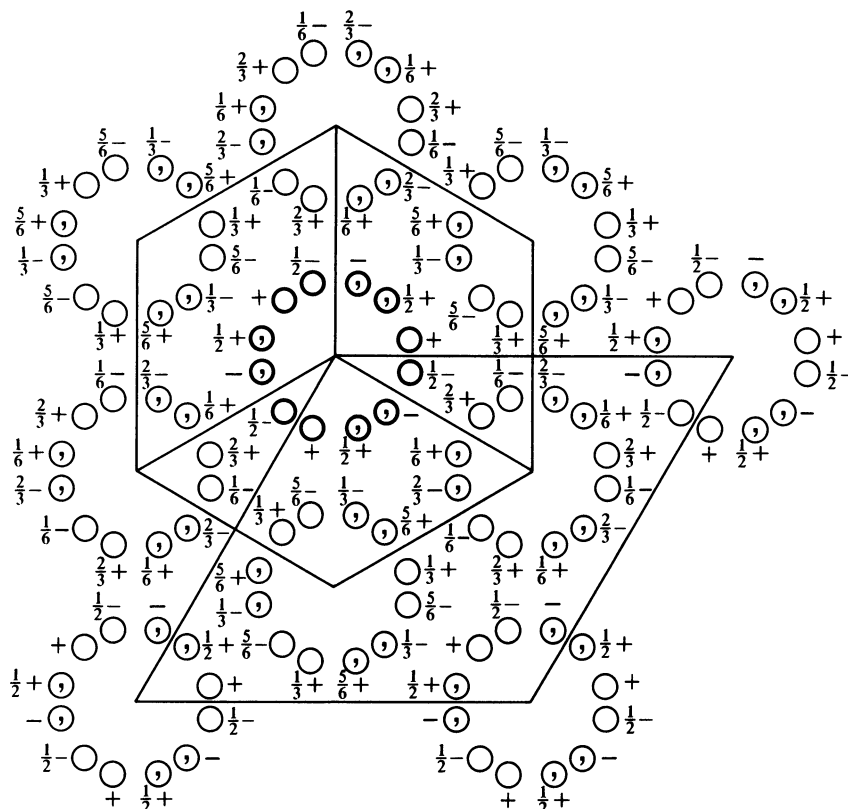
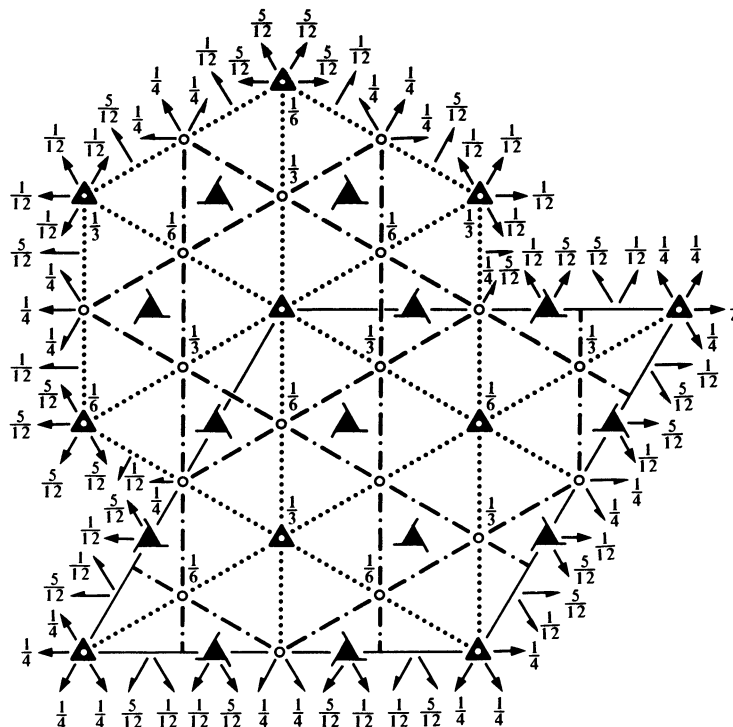
Trigonal

No. 167

$R\bar{3}2/c$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin at centre ($\bar{3}$) at $\bar{3}c$

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$
Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- | | | |
|-------------------------|------------------------------|------------------------------|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) $2 x,x,\frac{1}{4}$ | (5) $2 x,0,\frac{1}{4}$ | (6) $2 0,y,\frac{1}{4}$ |
| (7) $\bar{1} 0,0,0$ | (8) $\bar{3}^+ 0,0,z; 0,0,0$ | (9) $\bar{3}^- 0,0,z; 0,0,0$ |
| (10) $c x,\bar{x},z$ | (11) $c x,2x,z$ | (12) $c 2x,x,z$ |

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ + set

- | | | |
|--|--|--|
| (1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ | (2) $3^+(0,0,\frac{1}{3}) \frac{1}{3},\frac{1}{3},z$ | (3) $3^-(0,0,\frac{1}{3}) \frac{1}{3},0,z$ |
| (4) $2(\frac{1}{2},\frac{1}{2},0) x,x-\frac{1}{6},\frac{5}{12}$ | (5) $2(\frac{1}{2},0,0) x,\frac{1}{6},\frac{5}{12}$ | (6) $2 \frac{1}{3},y,\frac{5}{12}$ |
| (7) $\bar{1} \frac{1}{3},\frac{1}{6},\frac{1}{6}$ | (8) $\bar{3}^+ \frac{1}{3},-\frac{1}{3},z; \frac{1}{3},-\frac{1}{3},\frac{1}{6}$ | (9) $\bar{3}^- \frac{1}{3},\frac{2}{3},z; \frac{1}{3},\frac{2}{3},\frac{1}{6}$ |
| (10) $g(\frac{1}{6},-\frac{1}{6},\frac{2}{6}) x+\frac{1}{2},\bar{x},z$ | (11) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6}) x+\frac{1}{4},2x,z$ | (12) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6}) 2x,x,z$ |

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ + set

- | | | |
|--|--|--|
| (1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ | (2) $3^+(0,0,\frac{2}{3}) 0,\frac{1}{3},z$ | (3) $3^-(0,0,\frac{2}{3}) \frac{1}{3},\frac{1}{3},z$ |
| (4) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{6},\frac{1}{12}$ | (5) $2 x,\frac{1}{3},\frac{1}{12}$ | (6) $2(0,\frac{1}{2},0) \frac{1}{6},y,\frac{1}{12}$ |
| (7) $\bar{1} \frac{1}{6},\frac{1}{3},\frac{1}{3}$ | (8) $\bar{3}^+ \frac{2}{3},\frac{1}{3},z; \frac{2}{3},\frac{1}{3},\frac{1}{3}$ | (9) $\bar{3}^- -\frac{1}{3},\frac{1}{3},z; -\frac{1}{3},\frac{1}{3},\frac{1}{3}$ |
| (10) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6}) x+\frac{1}{2},\bar{x},z$ | (11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6}) x,2x,z$ | (12) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6}) 2x-\frac{1}{2},x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)$ + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ +

Reflection conditions

General:

- | | | | |
|---------------|--------------------------------------|---------------------------------------|---|
| 36 <i>f</i> 1 | (1) x,y,z | (2) $\bar{y},x-y,z$ | (3) $\bar{x}+y,\bar{x},z$ |
| | (4) $y,x,\bar{z}+\frac{1}{2}$ | (5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ | (6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ |
| | (7) \bar{x},\bar{y},\bar{z} | (8) $y,\bar{x}+y,\bar{z}$ | (9) $x-y,x,\bar{z}$ |
| | (10) $\bar{y},\bar{x},z+\frac{1}{2}$ | (11) $\bar{x}+y,y,z+\frac{1}{2}$ | (12) $x,x-y,z+\frac{1}{2}$ |

- $hkil : -h+k+l=3n$
 $hki0 : -h+k=3n$
 $hh\bar{2}hl : l=3n$
 $h\bar{h}0l : h+l=3n, l=2n$
 $000l : l=6n$
 $h\bar{h}00 : h=3n$

Special: as above, plus

- | | | | | | | |
|------------------------|-------------------|---------------------------|-------------------------------|-----------------------------|-----------------------------|---------------------------------------|
| 18 <i>e</i> .2 | $x,0,\frac{1}{4}$ | $0,x,\frac{1}{4}$ | $\bar{x},\bar{x},\frac{1}{4}$ | $\bar{x},0,\frac{3}{4}$ | $0,\bar{x},\frac{3}{4}$ | $x,x,\frac{3}{4}$ |
| 18 <i>d</i> $\bar{1}$ | $\frac{1}{2},0,0$ | $0,\frac{1}{2},0$ | $\frac{1}{2},\frac{1}{2},0$ | $0,\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},0,\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ |
| 12 <i>c</i> 3. | $0,0,z$ | $0,0,\bar{z}+\frac{1}{2}$ | $0,0,\bar{z}$ | $0,0,z+\frac{1}{2}$ | | |
| 6 <i>b</i> $\bar{3}$. | $0,0,0$ | $0,0,\frac{1}{2}$ | | | | |
| 6 <i>a</i> 32 | $0,0,\frac{1}{4}$ | $0,0,\frac{3}{4}$ | | | | |

- no extra conditions
 $hkil : l=2n$
 $hkil : l=2n$
 $hkil : l=2n$
 $hkil : l=2n$

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$
 Origin at 0,0,z

Along [100] $p2$

$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} + 4\mathbf{b} + \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$
 Origin at $x,0,0$

Along [210] $p2gm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
 Origin at $x,\frac{1}{2}x,0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I	[2] $R\bar{3}c$ (161)	(1; 2; 3; 10; 11; 12)+
	[2] $R\bar{3}2$ (155)	(1; 2; 3; 4; 5; 6)+
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	(1; 2; 3; 7; 8; 9)+
	{ [3] $R12/c$ ($C2/c$, 15)	(1; 4; 7; 10)+
	{ [3] $R12/c$ ($C2/c$, 15)	(1; 5; 7; 11)+
	{ [3] $R12/c$ ($C2/c$, 15)	(1; 6; 7; 12)+
IIa	{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
	{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc	[4] $R\bar{3}c$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 5\mathbf{c}$) (167)
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Minimal non-isomorphic supergroups

I	[4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)
II	[2] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (166); [3] $P\bar{3}1c$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (163)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I	[2] $R\bar{3}c$ (161)	1; 2; 3; 10; 11; 12
	[2] $R\bar{3}2$ (155)	1; 2; 3; 4; 5; 6
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	1; 2; 3; 7; 8; 9
	{ [3] $R12/c$ ($C2/c$, 15)	1; 4; 7; 10
	{ [3] $R12/c$ ($C2/c$, 15)	1; 5; 7; 11
	{ [3] $R12/c$ ($C2/c$, 15)	1; 6; 7; 12

IIa none

IIb	[3] $P\bar{3}c1$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$) (165)
------------	---

Maximal isomorphic subgroups of lowest index

IIc	[4] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b} + 2\mathbf{c}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b} + 2\mathbf{c}, \mathbf{c}' = 2\mathbf{a} + 2\mathbf{b} + \mathbf{c}$) (167)
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Minimal non-isomorphic supergroups

I	[4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)
II	[2] $R\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}), \mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}), \mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$) (166); [3] $P\bar{3}1c$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$) (163)

Trigonal

$\bar{3}m$

D_{3d}^6

$R\bar{3}c$

Patterson symmetry $R\bar{3}m$

$R\bar{3}2/c$

No. 167

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

Origin at centre ($\bar{3}$) at $\bar{3}c$

Asymmetric unit $\frac{1}{4} \leq x \leq \frac{5}{4}; \frac{1}{4} \leq y \leq \frac{5}{4}; \frac{1}{4} \leq z \leq \frac{3}{4}; y \leq x; z \leq \min(y, \frac{3}{2} - x)$

Vertices $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{5}{4}, \frac{1}{4}, \frac{1}{4}; \frac{5}{4}, \frac{5}{4}, \frac{1}{4}; \frac{3}{4}, \frac{3}{4}, \frac{3}{4}$

Symmetry operations

- | | | |
|---|---|---|
| (1) 1 | (2) $3^+ x, x, x$ | (3) $3^- x, x, x$ |
| (4) $2 \bar{x} + \frac{1}{2}, \frac{1}{4}, x$ | (5) $2 x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ | (6) $2 \frac{1}{4}, y + \frac{1}{2}, \bar{y}$ |
| (7) $\bar{1} 0, 0, 0$ | (8) $\bar{3}^+ x, x, x; 0, 0, 0$ | (9) $\bar{3}^- x, x, x; 0, 0, 0$ |
| (10) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, x$ | (11) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, z$ | (12) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, y$ |

Generators selected (1); $t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); (2); (4); (7)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions			
12 <i>f</i> 1	(1) x, y, z (4) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (10) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	(2) z, x, y (5) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{z}, \bar{x}, \bar{y}$ (11) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(3) y, z, x (6) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (9) $\bar{y}, \bar{z}, \bar{x}$ (12) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	General: $hhl : l = 2n$ $hhh : h = 2n$ Special: as above, plus no extra conditions			
6 <i>e</i> .2	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, x, \bar{x} + \frac{1}{2}$ $\frac{3}{4}, \bar{x}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ $x + \frac{1}{2}, \frac{3}{4}, \bar{x}$	$hkl : h + k + l = 2n$			
6 <i>d</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>c</i> 3.	x, x, x	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{x}, \bar{x}$	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$		
2 <i>b</i> $\bar{3}$.	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$				
2 <i>a</i> 32	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$				

Symmetry of special projections

Along $[111] p6mm$

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$

Origin at x, x, x

(Continued on preceding page)

Along $[1\bar{1}0] p2$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, \bar{x}, 0$

Along $[2\bar{1}\bar{1}] p2gm$

$\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$

Origin at $2x, \bar{x}, \bar{x}$

$P6$

C_6^1

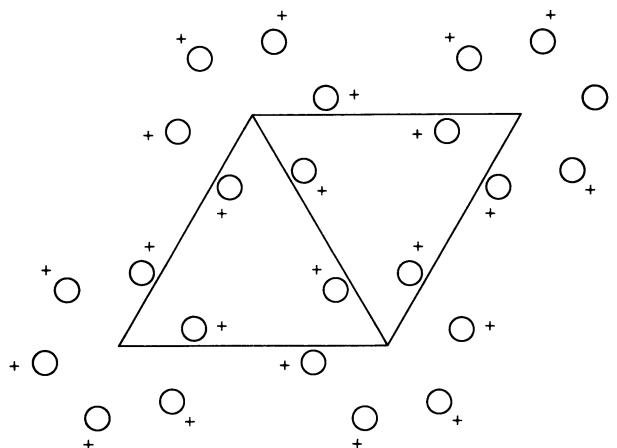
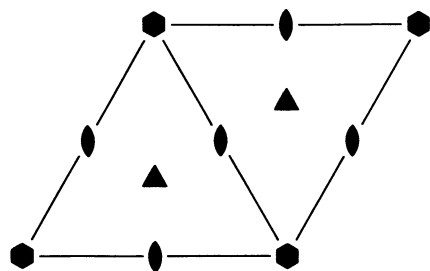
6

Hexagonal

No. 168

$P6$

Patterson symmetry $P6/m$



Origin on 6

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1; x \leq (1+y)/2; y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, 1$ $\frac{1}{2}, 0, 1$ $\frac{2}{3}, \frac{1}{3}, 1$ $\frac{1}{2}, \frac{1}{2}, 1$

Symmetry operations

(1) 1 (2) 3^+ $0, 0, z$ (3) 3^- $0, 0, z$
 (4) 2 $0, 0, z$ (5) 6^- $0, 0, z$ (6) 6^+ $0, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
6 <i>d</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) \bar{x}, \bar{y}, z (5) $y, \bar{x} + y, z$ (6) $x - y, x, z$	General: no conditions Special: no extra conditions
3 <i>c</i> 2..	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, z$	
2 <i>b</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z$	
1 <i>a</i> 6..	$0, 0, z$	

Symmetry of special projections

Along $[001]$ $p6$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[210]$ $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I $[2]P3(143)$ 1; 2; 3
 $[3]P2(3)$ 1; 4

IIa none

IIb $[2]P6_3(\mathbf{c}' = 2\mathbf{c})(173)$; $[3]P6_4(\mathbf{c}' = 3\mathbf{c})(172)$; $[3]P6_2(\mathbf{c}' = 3\mathbf{c})(171)$

Maximal isomorphic subgroups of lowest index

IIc $[2]P6(\mathbf{c}' = 2\mathbf{c})(168)$; $[3]H6(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})(P6, 168)$

Minimal non-isomorphic supergroups

I $[2]P6/m(175)$; $[2]P622(177)$; $[2]P6mm(183)$; $[2]P6cc(184)$

II none

$P6_1$

C_6^2

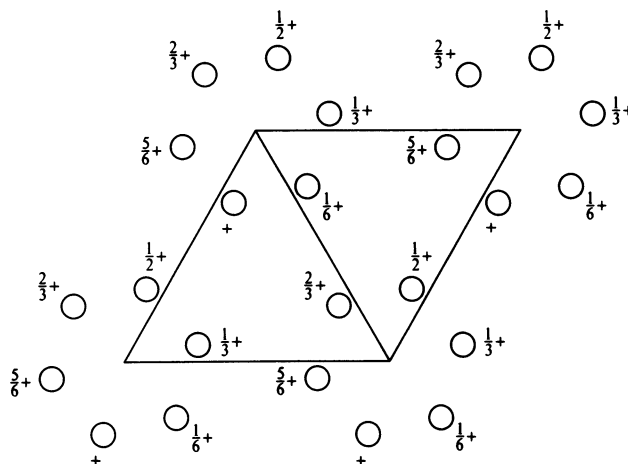
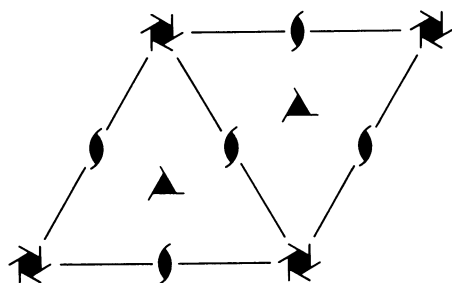
6

Hexagonal

No. 169

$P6_1$

Patterson symmetry $P6/m$



Origin on 6_1

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$

Vertices $0, 0, 0$ $1, 0, 0$ $1, 1, 0$ $0, 1, 0$
 $0, 0, \frac{1}{6}$ $1, 0, \frac{1}{6}$ $1, 1, \frac{1}{6}$ $0, 1, \frac{1}{6}$

Symmetry operations

- (1) 1 (2) $3^+(0, 0, \frac{1}{3})$ $0, 0, z$ (3) $3^-(0, 0, \frac{2}{3})$ $0, 0, z$
 (4) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (5) $6^-(0, 0, \frac{5}{6})$ $0, 0, z$ (6) $6^+(0, 0, \frac{1}{6})$ $0, 0, z$

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
6 <i>a</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z + \frac{1}{3}$ (3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{5}{6}$ (6) $x - y, x, z + \frac{1}{6}$	General: $000l : l = 6n$

Symmetry of special projections

Along $[001]$ $p6$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p1g1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[210]$ $p1g1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

- I** $[2] P3_1(144)$ 1; 2; 3
 $[3] P2_1(4)$ 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

- IIc** $[3] H6_1(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})(P6_1, 169)$; $[5] P6_5(\mathbf{c}' = 5\mathbf{c})(170)$; $[7] P6_1(\mathbf{c}' = 7\mathbf{c})(169)$

Minimal non-isomorphic supergroups

- I** $[2] P6_2(178)$

- II** $[2] P6_2(\mathbf{c}' = \frac{1}{2}\mathbf{c})(171)$; $[3] P6_3(\mathbf{c}' = \frac{1}{3}\mathbf{c})(173)$

Hexagonal

6

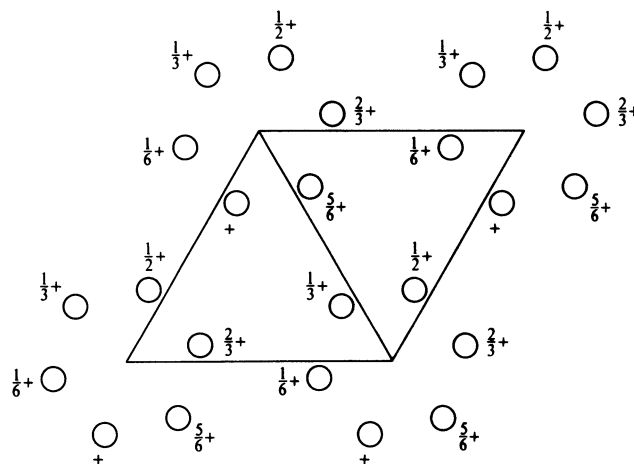
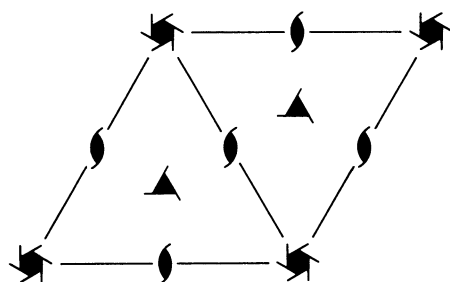
C_6^3

$P6_5$

Patterson symmetry $P6/m$

$P6_5$

No. 170



Origin on 6₅

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}$
 Vertices $0, 0, 0$ $1, 0, 0$ $1, 1, 0$ $0, 1, 0$
 $0, 0, \frac{1}{6}$ $1, 0, \frac{1}{6}$ $1, 1, \frac{1}{6}$ $0, 1, \frac{1}{6}$

Symmetry operations

- (1) 1 (2) $3^+(0, 0, \frac{2}{3})$ $0, 0, z$ (3) $3^-(0, 0, \frac{1}{3})$ $0, 0, z$
 (4) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (5) $6^-(0, 0, \frac{1}{6})$ $0, 0, z$ (6) $6^+(0, 0, \frac{5}{6})$ $0, 0, z$

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
6 <i>a</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z + \frac{2}{3}$ (3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{1}{6}$ (6) $x - y, x, z + \frac{5}{6}$	General: $000l : l = 6n$

Symmetry of special projections

Along $[001]$ $p6$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$	Along $[100]$ $p1g1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$	Along $[210]$ $p1g1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
--	---	--

Maximal non-isomorphic subgroups

- I** $[2]P3_2(145)$ 1; 2; 3
 $[3]P2_1(4)$ 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

- IIc** $[3]H6_5$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_5, 170$); $[5]P6_1$ ($\mathbf{c}' = 5\mathbf{c}$) (169); $[7]P6_5$ ($\mathbf{c}' = 7\mathbf{c}$) (170)

Minimal non-isomorphic supergroups

- I** $[2]P6_5 22$ (179)

- II** $[2]P6_4$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (172); $[3]P6_3$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (173)

$P6_2$

C_6^4

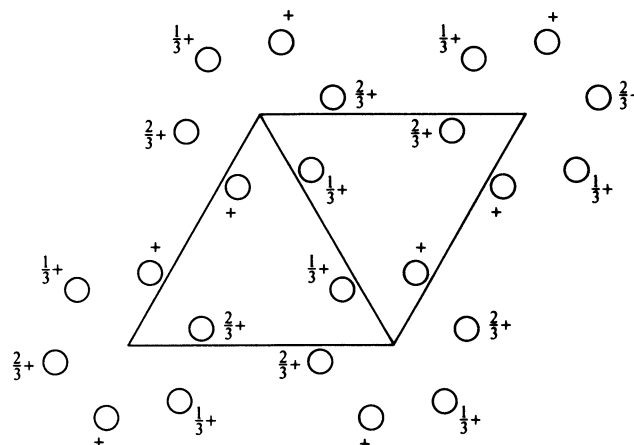
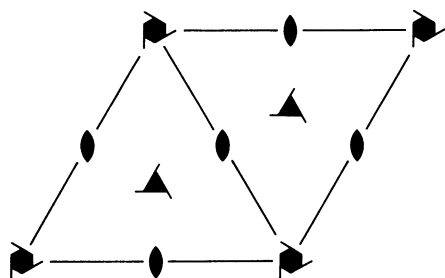
6

Hexagonal

No. 171

$P6_2$

Patterson symmetry $P6/m$



Origin on 2 on 6_2

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{3}; y \leq x$
 Vertices $0,0,0$ $1,0,0$ $1,1,0$
 $0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$

Symmetry operations

- (1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
 (4) 2 $0,0,z$ (5) $6^-(0,0,\frac{2}{3})$ $0,0,z$ (6) $6^+(0,0,\frac{1}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
6 <i>c</i> 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (4) \bar{x},\bar{y},z (5) $y,\bar{x}+y,z+\frac{2}{3}$ (6) $x-y,x,z+\frac{1}{3}$	General: $000l : l = 3n$ Special: as above, plus $hkil : h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$ $hkil : l = 3n$
3 <i>b</i> 2..	$\frac{1}{2},\frac{1}{2},z$ $\frac{1}{2},0,z+\frac{2}{3}$ $0,\frac{1}{2},z+\frac{1}{3}$	
3 <i>a</i> 2..	$0,0,z$ $0,0,z+\frac{2}{3}$ $0,0,z+\frac{1}{3}$	

Symmetry of special projections

Along $[001]$ $p6$ Along $[100]$ $p1m1$ Along $[210]$ $p1m1$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $0,0,0$ Origin at $x,0,0$ Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

- I** $[2]P3_2(145)$ 1; 2; 3 **IIa** none
 $[3]P2(3)$ 1; 4 **IIb** $[2]P6_1(c' = 2c)(169)$

Maximal isomorphic subgroups of lowest index

IIc $[2]P6_4(c' = 2c)(172)$; $[3]H6_2(a' = 3a, b' = 3b)(P6_2, 171)$; $[7]P6_2(c' = 7c)(171)$

Minimal non-isomorphic supergroups

- I** $[2]P6_222(180)$
II $[3]P6(c' = \frac{1}{3}c)(168)$

Hexagonal

6

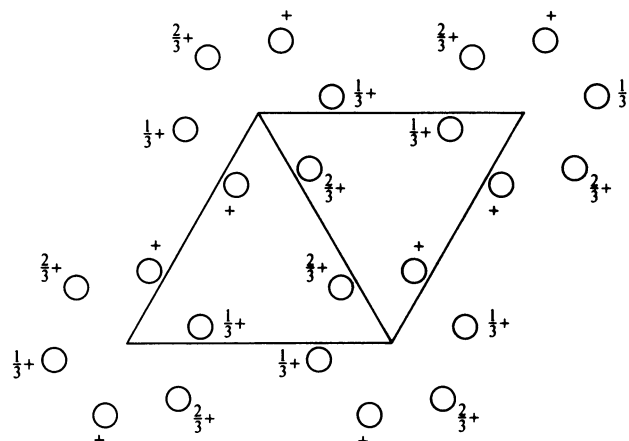
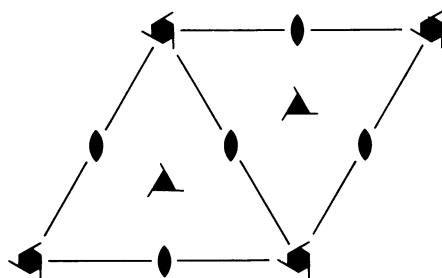
C_6^5

$P6_4$

Patterson symmetry $P6/m$

$P6_4$

No. 172



Origin on 2 on 6_4

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{3}; y \leq x$
 Vertices $0,0,0$ $1,0,0$ $1,1,0$
 $0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$

Symmetry operations

- (1) 1
- (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$
- (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
- (4) 2 $0,0,z$
- (5) $6^-(0,0,\frac{1}{3})$ $0,0,z$
- (6) $6^+(0,0,\frac{2}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
6 <i>c</i> 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{1}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (4) \bar{x},\bar{y},z (5) $y,\bar{x}+y,z+\frac{1}{3}$ (6) $x-y,x,z+\frac{2}{3}$	General: $000l : l = 3n$ Special: as above, plus $hkil : h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$ $hkil : l = 3n$
3 <i>b</i> 2..	$\frac{1}{2},\frac{1}{2},z$ $\frac{1}{2},0,z+\frac{1}{3}$ $0,\frac{1}{2},z+\frac{2}{3}$	
3 <i>a</i> 2..	$0,0,z$ $0,0,z+\frac{1}{3}$ $0,0,z+\frac{2}{3}$	

Symmetry of special projections

Along [001] $p6$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,0$
 Along [100] $p1m1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,0$
 Along [210] $p1m1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

- I [2] $P3_1(144)$ 1; 2; 3
- [3] $P2(3)$ 1; 4
- IIa none
- IIb [2] $P6_5(c' = 2c)$ (170)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_2(c' = 2c)$ (171); [3] $H6_4(a' = 3a, b' = 3b)$ ($P6_4, 172$); [7] $P6_4(c' = 7c)$ (172)

Minimal non-isomorphic supergroups

- I [2] $P6_422$ (181)
- II [3] $P6(c' = \frac{1}{3}c)$ (168)

$P6_3$

C_6^6

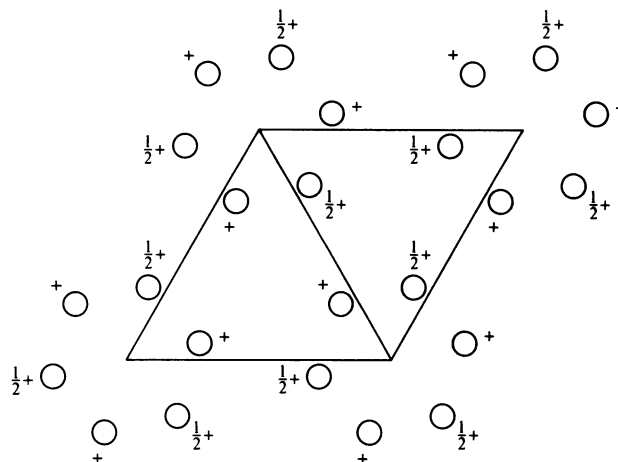
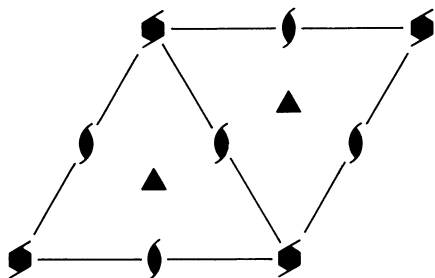
6

Hexagonal

No. 173

$P6_3$

Patterson symmetry $P6/m$



Origin on 3 on 6_3

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1
 (2) $3^+ 0, 0, z$
 (3) $3^- 0, 0, z$
 (4) $2(0, 0, \frac{1}{2}) 0, 0, z$
 (5) $6^-(0, 0, \frac{1}{2}) 0, 0, z$
 (6) $6^+(0, 0, \frac{1}{2}) 0, 0, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 <i>c</i> 1	(1) x, y, z (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z + \frac{1}{2}$	General: $000l : l = 2n$ Special: as above, plus $hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$ $hkil : l = 2n$
2 <i>b</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$		
2 <i>a</i> 3..	$0, 0, z$	$0, 0, z + \frac{1}{2}$		

Symmetry of special projections

Along $[001]$ $p6$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p1g1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[210]$ $p1g1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [2] $P3$ (143) 1; 2; 3
 [3] $P2_1$ (4) 1; 4

IIa none

IIb [3] $P6_5$ ($\mathbf{c}' = 3\mathbf{c}$) (170); [3] $P6_1$ ($\mathbf{c}' = 3\mathbf{c}$) (169)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3$ ($\mathbf{c}' = 3\mathbf{c}$) (173); [3] $H6_3$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3$, 173)

Minimal non-isomorphic supergroups

I [2] $P6_3/m$ (176); [2] $P6_3 22$ (182); [2] $P6_3 cm$ (185); [2] $P6_3 mc$ (186)

II [2] $P6$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (168)

$P\bar{6}$

C_{3h}^1

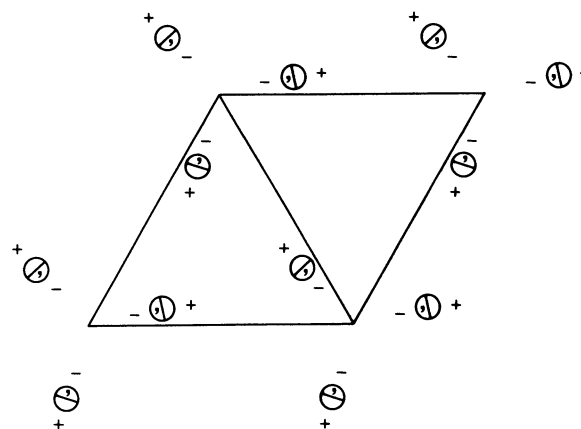
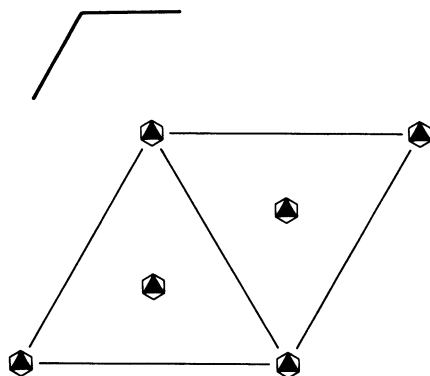
$\bar{6}$

Hexagonal

No. 174

$P\bar{6}$

Patterson symmetry $P6/m$



Origin at $\bar{6}$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1 (2) 3^+ $0, 0, z$ (3) 3^- $0, 0, z$
 (4) m $x, y, 0$ (5) $\bar{6}^-$ $0, 0, z; 0, 0, 0$ (6) $\bar{6}^+$ $0, 0, z; 0, 0, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
6	l 1	(1) x, y, z (4) x, y, \bar{z}	(2) $\bar{y}, x - y, z$ (5) $\bar{y}, x - y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x} + y, \bar{x}, \bar{z}$	General: no conditions Special: no extra conditions
3	k $m..$	$x, y, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$	
3	j $m..$	$x, y, 0$	$\bar{y}, x - y, 0$	$\bar{x} + y, \bar{x}, 0$	
2	i $3..$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$		
2	h $3..$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$		
2	g $3..$	$0, 0, z$	$0, 0, \bar{z}$		
1	f $\bar{6}..$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$			
1	e $\bar{6}..$	$\frac{2}{3}, \frac{1}{3}, 0$			
1	d $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$			
1	c $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, 0$			
1	b $\bar{6}..$	$0, 0, \frac{1}{2}$			
1	a $\bar{6}..$	$0, 0, 0$			

Symmetry of special projections

Along $[001]$ $p3$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[100]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along $[210]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I $[2] P3 (143)$ 1; 2; 3
 $[3] Pm (6)$ 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2] P\bar{6} (\mathbf{c}' = 2\mathbf{c}) (174)$; $[3] H\bar{6} (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (P\bar{6}, 174)$

Minimal non-isomorphic supergroups

I $[2] P6/m (175)$; $[2] P6_3/m (176)$; $[2] P\bar{6}m2 (187)$; $[2] P\bar{6}c2 (188)$; $[2] P\bar{6}2m (189)$; $[2] P\bar{6}2c (190)$

II none

$P6/m$

C_{6h}^1

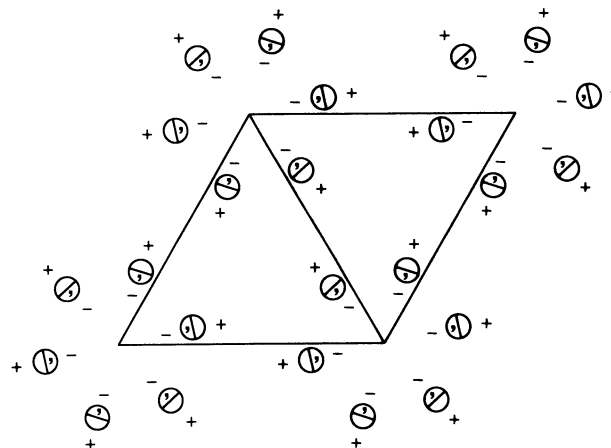
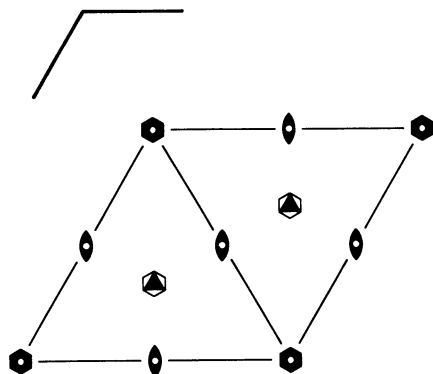
$6/m$

Hexagonal

No. 175

$P6/m$

Patterson symmetry $P6/m$



Origin at centre ($6/m$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|-------------------------|--|--|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) 2 $0, 0, z$ | (5) 6^- $0, 0, z$ | (6) 6^+ $0, 0, z$ |
| (7) $\bar{1}$ $0, 0, 0$ | (8) $\bar{3}^+$ $0, 0, z$; $0, 0, 0$ | (9) $\bar{3}^-$ $0, 0, z$; $0, 0, 0$ |
| (10) m $x, y, 0$ | (11) $\bar{6}^-$ $0, 0, z$; $0, 0, 0$ | (12) $\bar{6}^+$ $0, 0, z$; $0, 0, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions		
				General:		
12 <i>l</i> 1	(1) x, y, z (4) \bar{x}, \bar{y}, z (7) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z}	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z$ (8) $y, \bar{x} + y, \bar{z}$ (11) $\bar{y}, x - y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z$ (9) $x - y, x, \bar{z}$ (12) $\bar{x} + y, \bar{x}, \bar{z}$	no conditions		
				Special: no extra conditions		
6 <i>k</i> $m..$	$x, y, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$	$y, \bar{x} + y, \frac{1}{2}$	$x - y, x, \frac{1}{2}$
6 <i>j</i> $m..$	$x, y, 0$	$\bar{y}, x - y, 0$	$\bar{x} + y, \bar{x}, 0$	$\bar{x}, \bar{y}, 0$	$y, \bar{x} + y, 0$	$x - y, x, 0$
6 <i>i</i> $2..$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$
4 <i>h</i> $3..$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$		
3 <i>g</i> $2/m..$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
3 <i>f</i> $2/m..$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2 <i>e</i> $6..$	$0, 0, z$	$0, 0, \bar{z}$				
2 <i>d</i> $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$				
2 <i>c</i> $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$				
1 <i>b</i> $6/m..$	$0, 0, \frac{1}{2}$					
1 <i>a</i> $6/m..$	$0, 0, 0$					

Symmetry of special projections

Along [001] $p6$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{6}$ (174) 1; 2; 3; 10; 11; 12
 [2] $P6$ (168) 1; 2; 3; 4; 5; 6
 [2] $P\bar{3}$ (147) 1; 2; 3; 7; 8; 9
 [3] $P2/m$ (10) 1; 4; 7; 10

IIa none

IIIb [2] $P6_3/m$ ($\mathbf{c}' = 2\mathbf{c}$) (176)

Maximal isomorphic subgroups of lowest index

IIIc [2] $P6/m$ ($\mathbf{c}' = 2\mathbf{c}$) (175); [3] $H6/m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6/m$, 175)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6/mcc$ (192)

II none

$P6_3/m$

C_{6h}^2

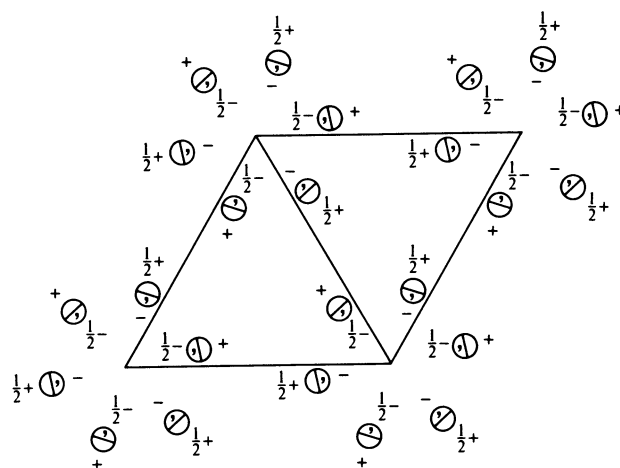
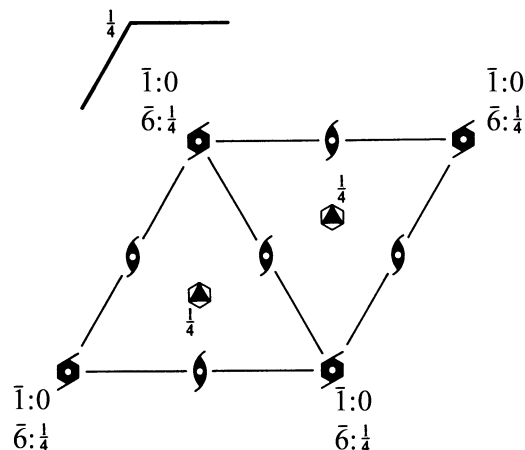
$6/m$

Hexagonal

No. 176

$P6_3/m$

Patterson symmetry $P6/m$



Origin at centre ($\bar{3}$) on 6_3

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{4}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|------------------------------------|---|---|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2}) 0, 0, z$ | (5) $6^-(0, 0, \frac{1}{2}) 0, 0, z$ | (6) $6^+(0, 0, \frac{1}{2}) 0, 0, z$ |
| (7) $\bar{1} 0, 0, 0$ | (8) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (9) $\bar{3}^- 0, 0, z; 0, 0, 0$ |
| (10) $m x, y, \frac{1}{4}$ | (11) $\bar{6}^- 0, 0, z; 0, 0, \frac{1}{4}$ | (12) $\bar{6}^+ 0, 0, z; 0, 0, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
12	<i>i</i> 1	(1) x, y, z (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (10) $x, y, \bar{z} + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (8) $y, \bar{x} + y, \bar{z}$ (11) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z + \frac{1}{2}$ (9) $x - y, x, \bar{z}$ (12) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$				General: $000l : l = 2n$ Special: as above, plus
6	<i>h</i> $m..$	$x, y, \frac{1}{4}$	$\bar{y}, x - y, \frac{1}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$	$y, \bar{x} + y, \frac{3}{4}$	$x - y, x, \frac{3}{4}$	no extra conditions
6	<i>g</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil : l = 2n$
4	<i>f</i> $3..$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$			$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4	<i>e</i> $3..$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$			$hkil : l = 2n$
2	<i>d</i> $\bar{6}..$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$					$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2	<i>c</i> $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$					$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2	<i>b</i> $\bar{3}..$	$0, 0, 0$	$0, 0, \frac{1}{2}$					$hkil : l = 2n$
2	<i>a</i> $\bar{6}..$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					$hkil : l = 2n$

Symmetry of special projections

Along [001] $p6$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

- I** [2] $P\bar{6}$ (174) 1; 2; 3; 10; 11; 12
- [2] $P6_3$ (173) 1; 2; 3; 4; 5; 6
- [2] $P\bar{3}$ (147) 1; 2; 3; 7; 8; 9
- [3] $P2_1/m$ (11) 1; 4; 7; 10

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/m$ ($\mathbf{c}' = 3\mathbf{c}$) (176); [3] $H6_3/m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3/m$, 176)

Minimal non-isomorphic supergroups

- I** [2] $P6_3/mcm$ (193); [2] $P6_3/mmc$ (194)
- II** [2] $P6/m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (175)

*P*622

D_6^1

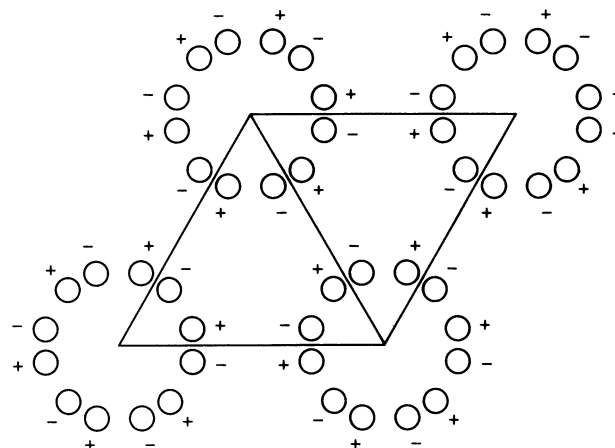
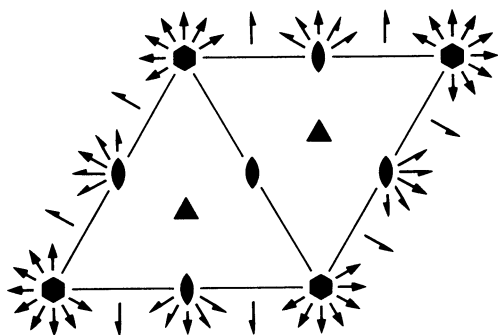
622

Hexagonal

No. 177

*P*622

Patterson symmetry *P*6/*m**m**m*



Origin at 622

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$

$0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|--------------------------------|--------------------------------|---------------------------------|
| (1) 1 | (2) 3^+ 0,0, <i>z</i> | (3) 3^- 0,0, <i>z</i> |
| (4) 2 0,0, <i>z</i> | (5) 6^- 0,0, <i>z</i> | (6) 6^+ 0,0, <i>z</i> |
| (7) 2 <i>x</i> , <i>x</i> ,0 | (8) 2 <i>x</i> ,0,0 | (9) 2 0, <i>y</i> ,0 |
| (10) 2 <i>x</i> , \bar{x} ,0 | (11) 2 <i>x</i> ,2 <i>x</i> ,0 | (12) 2 2 <i>x</i> , <i>x</i> ,0 |

Maximal isomorphic subgroups of lowest index

IIc [2] *P*622 (*c'* = 2*c*) (177); [3] *H*622 (*a'* = 3*a*, *b'* = 3*b*) (*P*622, 177)

Minimal non-isomorphic supergroups

I [2] *P*6/*m**m**m* (191); [2] *P*6/*m**c**c* (192)

II none

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

12	<i>n</i>	1	(1) x, y, z (4) \bar{x}, \bar{y}, z (7) y, x, \bar{z} (10) $\bar{y}, \bar{x}, \bar{z}$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z$ (8) $x - y, \bar{y}, \bar{z}$ (11) $\bar{x} + y, y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $x, x - y, \bar{z}$
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General:

no conditions

Special: no extra conditions

6	<i>m</i>	..2	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$
6	<i>l</i>	..2	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$
6	<i>k</i>	.2.	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$
6	<i>j</i>	.2.	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$
6	<i>i</i>	2..	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$
4	<i>h</i>	3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$		
3	<i>g</i>	222	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
3	<i>f</i>	222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	<i>e</i>	6..	$0, 0, z$	$0, 0, \bar{z}$				
2	<i>d</i>	3.2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$				
2	<i>c</i>	3.2	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$				
1	<i>b</i>	622	$0, 0, \frac{1}{2}$					
1	<i>a</i>	622	$0, 0, 0$					

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [210] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P611$ ($P6, 168$)	1; 2; 3; 4; 5; 6
	[2] $P321$ (150)	1; 2; 3; 7; 8; 9
	[2] $P312$ (149)	1; 2; 3; 10; 11; 12
	{ [3] $P222$ ($C222, 21$)	1; 4; 7; 10
	{ [3] $P222$ ($C222, 21$)	1; 4; 8; 11
	{ [3] $P222$ ($C222, 21$)	1; 4; 9; 12

IIa none

IIb [2] $P6_322$ ($\mathbf{c}' = 2\mathbf{c}$) (182); [3] $P6_422$ ($\mathbf{c}' = 3\mathbf{c}$) (181); [3] $P6_222$ ($\mathbf{c}' = 3\mathbf{c}$) (180)

(Continued on preceding page)

$P6_122$

D_6^2

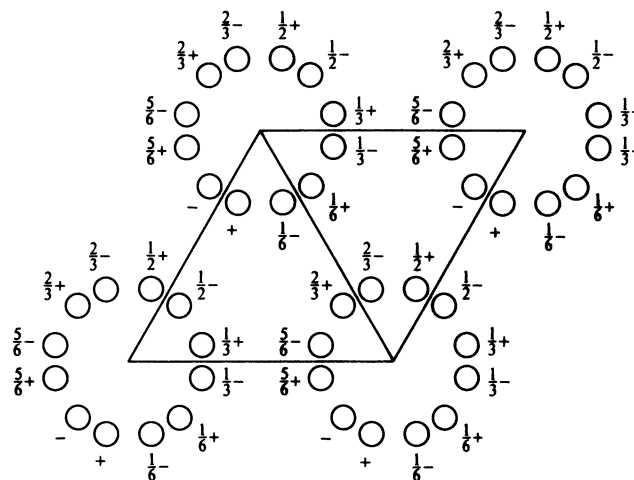
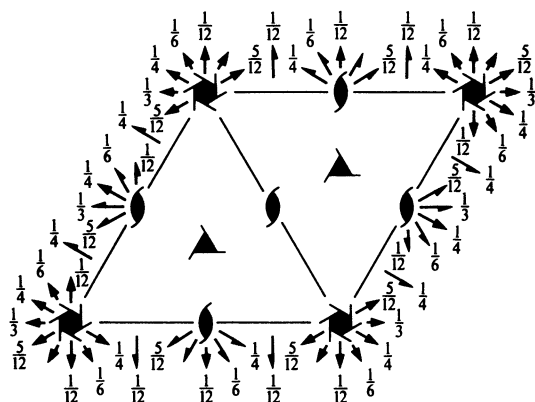
622

Hexagonal

No. 178

$P6_122$

Patterson symmetry $P6/mmm$



Origin on $2[100]$ at $6_1(2, 1, 1)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{12}$
 Vertices $0, 0, 0$ $1, 0, 0$ $1, 1, 0$ $0, 1, 0$
 $0, 0, \frac{1}{12}$ $1, 0, \frac{1}{12}$ $1, 1, \frac{1}{12}$ $0, 1, \frac{1}{12}$

Symmetry operations

- | | | |
|--------------------------------------|--|--|
| (1) 1 | (2) $3^+(0, 0, \frac{1}{3})$ $0, 0, z$ | (3) $3^-(0, 0, \frac{2}{3})$ $0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2})$ $0, 0, z$ | (5) $6^-(0, 0, \frac{5}{6})$ $0, 0, z$ | (6) $6^+(0, 0, \frac{1}{6})$ $0, 0, z$ |
| (7) 2 $x, x, \frac{1}{6}$ | (8) 2 $x, 0, 0$ | (9) 2 $0, y, \frac{1}{3}$ |
| (10) 2 $x, \bar{x}, \frac{5}{12}$ | (11) 2 $x, 2x, \frac{1}{4}$ | (12) 2 $2x, x, \frac{1}{12}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions					
								General:					
12 <i>c</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z + \frac{1}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$	(4) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(5) $y, \bar{x} + y, z + \frac{5}{6}$	(6) $x - y, x, z + \frac{1}{6}$	(7) $y, x, \bar{z} + \frac{1}{3}$	(8) $x - y, \bar{y}, \bar{z}$	(9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{2}{3}$	(10) $\bar{y}, \bar{x}, \bar{z} + \frac{5}{6}$	(11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$	(12) $x, x - y, \bar{z} + \frac{1}{6}$	000 <i>l</i> : $l = 6n$
								Special: as above, plus					
6 <i>b</i> . . 2	$x, 2x, \frac{1}{4}$	$2\bar{x}, \bar{x}, \frac{7}{12}$	$x, \bar{x}, \frac{11}{12}$	$\bar{x}, 2\bar{x}, \frac{3}{4}$	$2x, x, \frac{1}{12}$	$\bar{x}, x, \frac{5}{12}$				$hh\bar{2}hl$: $l = 2n$ or $l = 3n + 1$ or $l = 3n + 2$			
6 <i>a</i> . 2 .	$x, 0, 0$	$0, x, \frac{1}{3}$	$\bar{x}, \bar{x}, \frac{2}{3}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{5}{6}$	$x, x, \frac{1}{6}$				$h\bar{h}0l$: $l = 2n$ or $l = 3n + 1$ or $l = 3n + 2$			

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, \frac{1}{12}$

Maximal non-isomorphic subgroups

I	[2] $P6_111$ ($P6_1$, 169)	1; 2; 3; 4; 5; 6
	[2] $P3_121$ (152)	1; 2; 3; 7; 8; 9
	[2] $P3_112$ (151)	1; 2; 3; 10; 11; 12
	{ [3] $P2_122$ ($C222_1$, 20)	1; 4; 7; 10
	{ [3] $P2_122$ ($C222_1$, 20)	1; 4; 8; 11
	{ [3] $P2_122$ ($C222_1$, 20)	1; 4; 9; 12

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $H6_122$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_122$, 178); [5] $P6_122$ ($\mathbf{c}' = 5\mathbf{c}$) (179); [7] $P6_122$ ($\mathbf{c}' = 7\mathbf{c}$) (178)

Minimal non-isomorphic supergroups

I none

II [2] $P6_122$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (180); [3] $P6_122$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (182)

$P6_522$

D_6^3

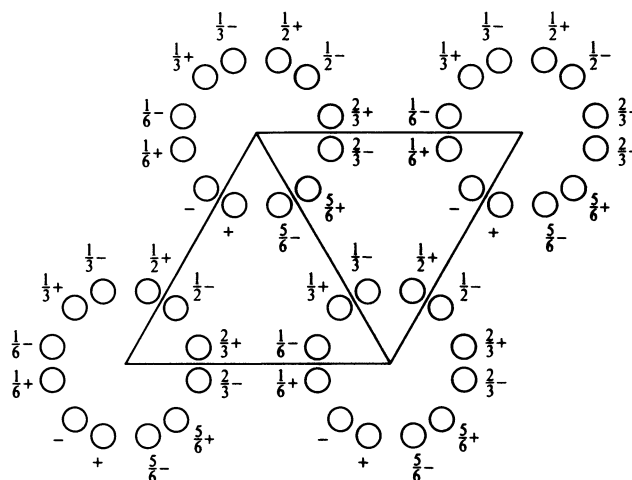
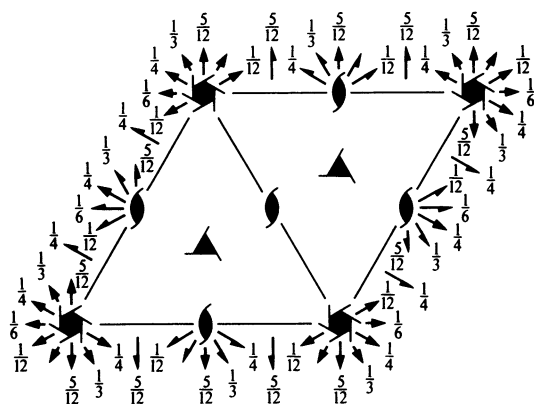
622

Hexagonal

No. 179

$P6_522$

Patterson symmetry $P6/mmm$



Origin on $2[100]$ at $6_5(2, 1, 1)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{12}$

Vertices $0, 0, 0 \quad 1, 0, 0 \quad 1, 1, 0 \quad 0, 1, 0$
 $0, 0, \frac{1}{12} \quad 1, 0, \frac{1}{12} \quad 1, 1, \frac{1}{12} \quad 0, 1, \frac{1}{12}$

Symmetry operations

- | | | | | |
|---|-----------------------------------|-----------|------------------------------------|-----------|
| (1) 1 | (2) $3^+(0, 0, \frac{2}{3})$ | $0, 0, z$ | (3) $3^-(0, 0, \frac{1}{3})$ | $0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2})$ | (5) $6^-(0, 0, \frac{1}{6})$ | $0, 0, z$ | (6) $6^+(0, 0, \frac{5}{6})$ | $0, 0, z$ |
| (7) $2 \quad x, x, \frac{1}{3}$ | (8) $2 \quad x, 0, 0$ | | (9) $2 \quad 0, y, \frac{1}{6}$ | |
| (10) $2 \quad x, \bar{x}, \frac{1}{12}$ | (11) $2 \quad x, 2x, \frac{1}{4}$ | | (12) $2 \quad 2x, x, \frac{5}{12}$ | |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions					
								General:					
12 <i>c</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z + \frac{2}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$	(4) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(5) $y, \bar{x} + y, z + \frac{1}{6}$	(6) $x - y, x, z + \frac{5}{6}$	(7) $y, x, \bar{z} + \frac{2}{3}$	(8) $x - y, \bar{y}, \bar{z}$	(9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{3}$	(10) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{6}$	(11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$	(12) $x, x - y, \bar{z} + \frac{5}{6}$	000 <i>l</i> : $l = 6n$
								Special: as above, plus					
6 <i>b</i> . . 2	$x, 2x, \frac{3}{4}$	$2\bar{x}, \bar{x}, \frac{5}{12}$	$x, \bar{x}, \frac{1}{12}$	$\bar{x}, 2\bar{x}, \frac{1}{4}$	$2x, x, \frac{11}{12}$	$\bar{x}, x, \frac{7}{12}$	$hh\bar{2}hl$: $l = 2n$ or $l = 3n + 1$ or $l = 3n + 2$						
6 <i>a</i> . 2 .	$x, 0, 0$	$0, x, \frac{2}{3}$	$\bar{x}, \bar{x}, \frac{1}{3}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{6}$	$x, x, \frac{5}{6}$	$h\bar{h}0l$: $l = 2n$ or $l = 3n + 1$ or $l = 3n + 2$						

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, \frac{5}{12}$

Maximal non-isomorphic subgroups

I	[2] $P6_511$ ($P6_5, 170$)	1; 2; 3; 4; 5; 6
	[2] $P3_221$ (154)	1; 2; 3; 7; 8; 9
	[2] $P3_212$ (153)	1; 2; 3; 10; 11; 12
	{ [3] $P2_122$ ($C222_1, 20$)	1; 4; 7; 10
	{ [3] $P2_122$ ($C222_1, 20$)	1; 4; 8; 11
	{ [3] $P2_122$ ($C222_1, 20$)	1; 4; 9; 12

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $H6_522$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_522, 179$); [5] $P6_122$ ($\mathbf{c}' = 5\mathbf{c}$) (178); [7] $P6_522$ ($\mathbf{c}' = 7\mathbf{c}$) (179)

Minimal non-isomorphic supergroups

I none

II [2] $P6_422$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (181); [3] $P6_322$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (182)

$P6_222$

D_6^4

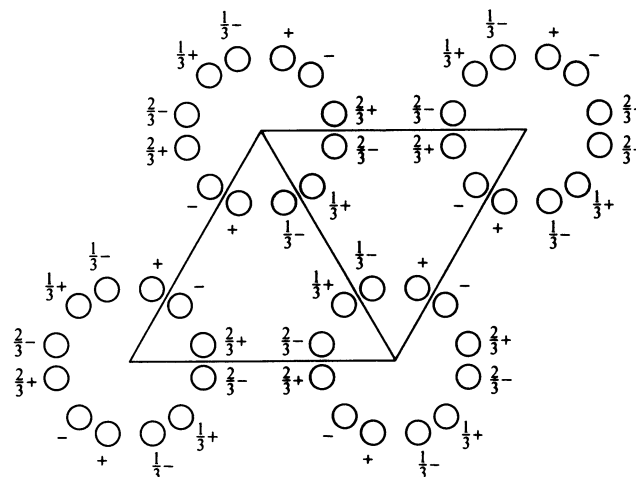
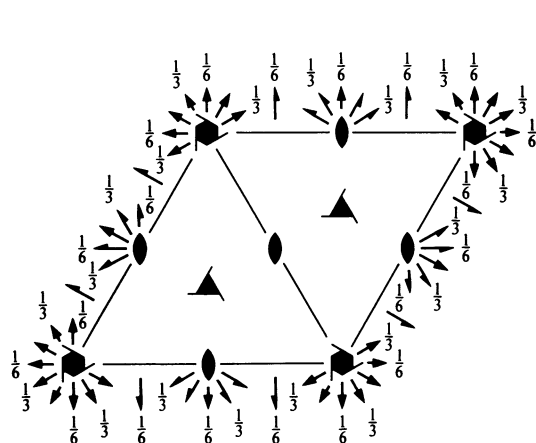
622

Hexagonal

No. 180

$P6_222$

Patterson symmetry $P6/mmm$



Origin at 222 at $6_2(2, 1, 1)(1, 2, 1)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}; y \leq x$
 Vertices $0, 0, 0 \quad 1, 0, 0 \quad 1, 1, 0$
 $0, 0, \frac{1}{6} \quad 1, 0, \frac{1}{6} \quad 1, 1, \frac{1}{6}$

Symmetry operations

- | | | |
|----------------------------------|--|--|
| (1) 1 | (2) $3^+(0, 0, \frac{2}{3}) \quad 0, 0, z$ | (3) $3^-(0, 0, \frac{1}{3}) \quad 0, 0, z$ |
| (4) 2 $0, 0, z$ | (5) $6^-(0, 0, \frac{2}{3}) \quad 0, 0, z$ | (6) $6^+(0, 0, \frac{1}{3}) \quad 0, 0, z$ |
| (7) 2 $x, x, \frac{1}{3}$ | (8) 2 $x, 0, 0$ | (9) 2 $0, y, \frac{1}{6}$ |
| (10) 2 $x, \bar{x}, \frac{1}{3}$ | (11) 2 $x, 2x, 0$ | (12) 2 $2x, x, \frac{1}{6}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>k</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z + \frac{2}{3}$ (3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$ (4) \bar{x}, \bar{y}, z (5) $y, \bar{x} + y, z + \frac{2}{3}$ (6) $x - y, x, z + \frac{1}{3}$ (7) $y, x, \bar{z} + \frac{2}{3}$ (8) $x - y, \bar{y}, \bar{z}$ (9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{3}$ (10) $\bar{y}, \bar{x}, \bar{z} + \frac{2}{3}$ (11) $\bar{x} + y, y, \bar{z}$ (12) $x, x - y, \bar{z} + \frac{1}{3}$	General: $000l : l = 3n$
		Special: as above, plus
6 <i>j</i> ..2	$x, 2x, \frac{1}{2}$ $2\bar{x}, \bar{x}, \frac{1}{6}$ $x, \bar{x}, \frac{5}{6}$ $\bar{x}, 2\bar{x}, \frac{1}{2}$ $2x, x, \frac{1}{6}$ $\bar{x}, x, \frac{5}{6}$	no extra conditions
6 <i>i</i> ..2	$x, 2x, 0$ $2\bar{x}, \bar{x}, \frac{2}{3}$ $x, \bar{x}, \frac{1}{3}$ $\bar{x}, 2\bar{x}, 0$ $2x, x, \frac{2}{3}$ $\bar{x}, x, \frac{1}{3}$	no extra conditions
6 <i>h</i> .2.	$x, 0, \frac{1}{2}$ $0, x, \frac{1}{6}$ $\bar{x}, \bar{x}, \frac{5}{6}$ $\bar{x}, 0, \frac{1}{2}$ $0, \bar{x}, \frac{1}{6}$ $x, x, \frac{5}{6}$	no extra conditions
6 <i>g</i> .2.	$x, 0, 0$ $0, x, \frac{2}{3}$ $\bar{x}, \bar{x}, \frac{1}{3}$ $\bar{x}, 0, 0$ $0, \bar{x}, \frac{2}{3}$ $x, x, \frac{1}{3}$	no extra conditions
6 <i>f</i> 2..	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z + \frac{2}{3}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{3}$ $0, \frac{1}{2}, \bar{z} + \frac{2}{3}$ $\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{3}$	$hkil : h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$
6 <i>e</i> 2..	$0, 0, z$ $0, 0, z + \frac{2}{3}$ $0, 0, z + \frac{1}{3}$ $0, 0, \bar{z} + \frac{2}{3}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{3}$	$hkil : l = 3n$
3 <i>d</i> 222	$\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{6}$ $\frac{1}{2}, \frac{1}{2}, \frac{5}{6}$	$hkil : h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$
3 <i>c</i> 222	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, \frac{2}{3}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{3}$	$hkil : h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$
3 <i>b</i> 222	$0, 0, \frac{1}{2}$ $0, 0, \frac{1}{6}$ $0, 0, \frac{5}{6}$	$hkil : l = 3n$
3 <i>a</i> 222	$0, 0, 0$ $0, 0, \frac{2}{3}$ $0, 0, \frac{1}{3}$	$hkil : l = 3n$

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at x, 0, 0

Along [210] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, \frac{1}{6}$

Maximal non-isomorphic subgroups

- I** [2] $P6_211$ ($P6_2$, 171) 1; 2; 3; 4; 5; 6
- [2] $P3_221$ (154) 1; 2; 3; 7; 8; 9
- [2] $P3_212$ (153) 1; 2; 3; 10; 11; 12
- { [3] $P222$ ($C222$, 21) 1; 4; 7; 10
- [3] $P222$ ($C222$, 21) 1; 4; 8; 11
- [3] $P222$ ($C222$, 21) 1; 4; 9; 12

IIa none

IIb [2] $P6_122$ ($\mathbf{c}' = 2\mathbf{c}$) (178)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_422$ ($\mathbf{c}' = 2\mathbf{c}$) (181); [3] $H6_222$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_222$, 180); [7] $P6_222$ ($\mathbf{c}' = 7\mathbf{c}$) (180)

Minimal non-isomorphic supergroups

I none

II [3] $P622$ ($\mathbf{c}' = \frac{1}{3}\mathbf{c}$) (177)

$P6_422$

D_6^5

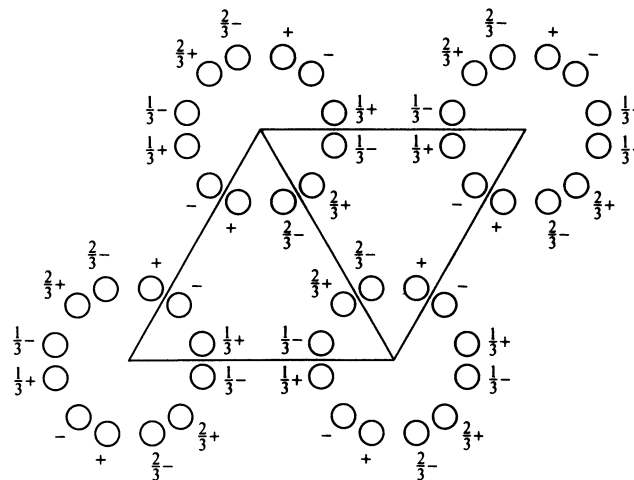
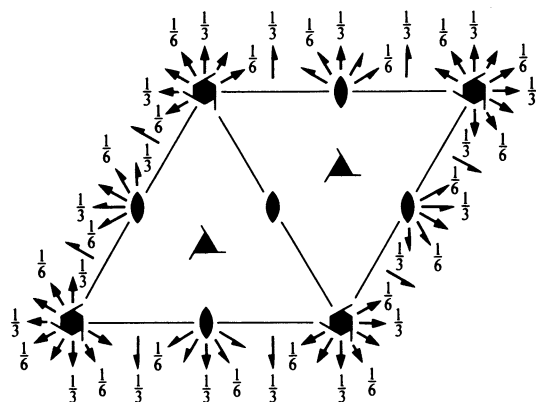
622

Hexagonal

No. 181

$P6_422$

Patterson symmetry $P6/mmm$



Origin at 222 at $6_4(2, 1, 1)(1, 2, 1)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}; y \leq x$
 Vertices $0, 0, 0 \quad 1, 0, 0 \quad 1, 1, 0$
 $0, 0, \frac{1}{6} \quad 1, 0, \frac{1}{6} \quad 1, 1, \frac{1}{6}$

Symmetry operations

- | | | |
|----------------------------------|--|--|
| (1) 1 | (2) $3^+(0, 0, \frac{1}{3})$ $0, 0, z$ | (3) $3^-(0, 0, \frac{2}{3})$ $0, 0, z$ |
| (4) 2 $0, 0, z$ | (5) $6^-(0, 0, \frac{1}{3})$ $0, 0, z$ | (6) $6^+(0, 0, \frac{2}{3})$ $0, 0, z$ |
| (7) 2 $x, x, \frac{1}{6}$ | (8) 2 $x, 0, 0$ | (9) 2 $0, y, \frac{1}{3}$ |
| (10) 2 $x, \bar{x}, \frac{1}{6}$ | (11) 2 $x, 2x, 0$ | (12) 2 $2x, x, \frac{1}{3}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions					
								General:					
12 <i>k</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z + \frac{1}{3}$	(3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$	(4) \bar{x}, \bar{y}, z	(5) $y, \bar{x} + y, z + \frac{1}{3}$	(6) $x - y, x, z + \frac{2}{3}$	(7) $y, x, \bar{z} + \frac{1}{3}$	(8) $x - y, \bar{y}, \bar{z}$	(9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{2}{3}$	(10) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{3}$	(11) $\bar{x} + y, y, \bar{z}$	(12) $x, x - y, \bar{z} + \frac{2}{3}$	000 <i>l</i> : $l = 3n$
								Special: as above, plus					
6 <i>j</i> ..2	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{5}{6}$	$x, \bar{x}, \frac{1}{6}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{5}{6}$	$\bar{x}, x, \frac{1}{6}$				no extra conditions			
6 <i>i</i> ..2	$x, 2x, 0$	$2\bar{x}, \bar{x}, \frac{1}{3}$	$x, \bar{x}, \frac{2}{3}$	$\bar{x}, 2\bar{x}, 0$	$2x, x, \frac{1}{3}$	$\bar{x}, x, \frac{2}{3}$				no extra conditions			
6 <i>h</i> .2.	$x, 0, \frac{1}{2}$	$0, x, \frac{5}{6}$	$\bar{x}, \bar{x}, \frac{1}{6}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{5}{6}$	$x, x, \frac{1}{6}$				no extra conditions			
6 <i>g</i> .2.	$x, 0, 0$	$0, x, \frac{1}{3}$	$\bar{x}, \bar{x}, \frac{2}{3}$	$\bar{x}, 0, 0$	$0, \bar{x}, \frac{1}{3}$	$x, x, \frac{2}{3}$				no extra conditions			
6 <i>f</i> 2..	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z + \frac{1}{3}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{2}{3}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{3}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{2}{3}$				$hkil$: $h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$			
6 <i>e</i> 2..	$0, 0, z$	$0, 0, z + \frac{1}{3}$	$0, 0, z + \frac{2}{3}$	$0, 0, \bar{z} + \frac{1}{3}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{2}{3}$				$hkil$: $l = 3n$			
3 <i>d</i> 222	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{5}{6}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{6}$							$hkil$: $h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$			
3 <i>c</i> 222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{3}$	$\frac{1}{2}, \frac{1}{2}, \frac{2}{3}$							$hkil$: $h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$			
3 <i>b</i> 222	$0, 0, \frac{1}{2}$	$0, 0, \frac{5}{6}$	$0, 0, \frac{1}{6}$							$hkil$: $l = 3n$			
3 <i>a</i> 222	$0, 0, 0$	$0, 0, \frac{1}{3}$	$0, 0, \frac{2}{3}$							$hkil$: $l = 3n$			

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, 0, 0

Along [210] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, \frac{1}{3}$

Maximal non-isomorphic subgroups

- I** [2] $P6_411 (P6_4, 172)$ 1; 2; 3; 4; 5; 6
 [2] $P3_121 (152)$ 1; 2; 3; 7; 8; 9
 [2] $P3_112 (151)$ 1; 2; 3; 10; 11; 12
 { [3] $P222 (C222, 21)$ 1; 4; 7; 10
 [3] $P222 (C222, 21)$ 1; 4; 8; 11
 [3] $P222 (C222, 21)$ 1; 4; 9; 12

IIa none

IIb [2] $P6_522 (c' = 2c) (179)$

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_222 (c' = 2c) (180)$; [3] $H6_422 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (P6_422, 181)$; [7] $P6_422 (c' = 7c) (181)$

Minimal non-isomorphic supergroups

I none

II [3] $P622 (c' = \frac{1}{3}c) (177)$

$P6_322$

D_6^6

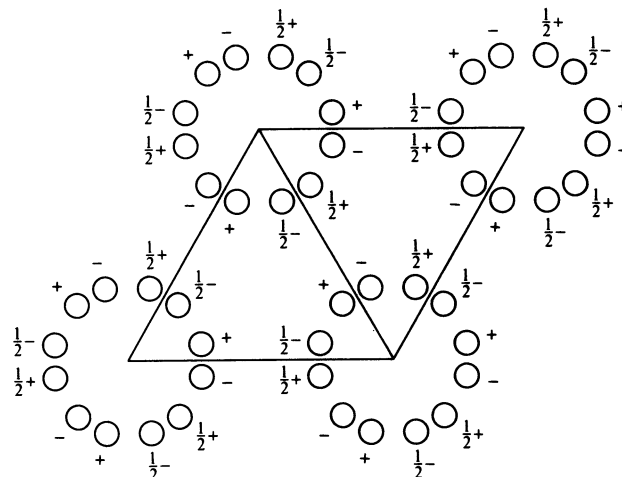
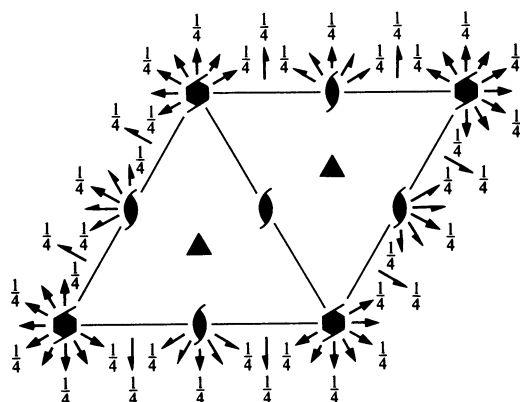
622

Hexagonal

No. 182

$P6_322$

Patterson symmetry $P6/mmm$



Origin at 321 at 6_321

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{4}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|------------------------------------|---------------------------------------|---------------------------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2}) 0, 0, z$ | (5) $6^- (0, 0, \frac{1}{2}) 0, 0, z$ | (6) $6^+ (0, 0, \frac{1}{2}) 0, 0, z$ |
| (7) $2 x, x, 0$ | (8) $2 x, 0, 0$ | (9) $2 0, y, 0$ |
| (10) $2 x, \bar{x}, \frac{1}{4}$ | (11) $2 x, 2x, \frac{1}{4}$ | (12) $2 2x, x, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>i</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (6) $x - y, x, z + \frac{1}{2}$ (7) y, x, \bar{z} (8) $x - y, \bar{y}, \bar{z}$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (10) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$ (12) $x, x - y, \bar{z} + \frac{1}{2}$	General: $000l : l = 2n$ Special: as above, plus
6 <i>h</i> . . 2	$x, 2x, \frac{1}{4}$ $2\bar{x}, \bar{x}, \frac{1}{4}$ $x, \bar{x}, \frac{1}{4}$ $\bar{x}, 2\bar{x}, \frac{3}{4}$ $2x, x, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	$hh\bar{2}hl : l = 2n$
6 <i>g</i> . 2 .	$x, 0, 0$ $0, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, 0, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $x, x, \frac{1}{2}$	$h\bar{h}0l : l = 2n$
4 <i>f</i> 3 . .	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$	$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> 3 . .	$0, 0, z$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$	$hkil : l = 2n$
2 <i>d</i> 3 . 2	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> 3 . 2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$hkil : l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>b</i> 3 . 2	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkil : l = 2n$
2 <i>a</i> 3 2 .	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkil : l = 2n$

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at 0, 0, z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $P6_311 (P6_3, 173)$	1; 2; 3; 4; 5; 6
	[2] $P321 (150)$	1; 2; 3; 7; 8; 9
	[2] $P312 (149)$	1; 2; 3; 10; 11; 12
	{ [3] $P2_122 (C222_1, 20)$	1; 4; 7; 10
	{ [3] $P2_122 (C222_1, 20)$	1; 4; 8; 11
	{ [3] $P2_122 (C222_1, 20)$	1; 4; 9; 12

IIa none

IIb [3] $P6_522 (\mathbf{c}' = 3\mathbf{c}) (179)$; [3] $P6_122 (\mathbf{c}' = 3\mathbf{c}) (178)$

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_322 (\mathbf{c}' = 3\mathbf{c}) (182)$; [3] $H6_322 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}) (P6_322, 182)$

Minimal non-isomorphic supergroups

I [2] $P6_3/mcm (193)$; [2] $P6_3/mmc (194)$

II [2] $P622 (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (177)$

$P6mm$

C_{6v}^1

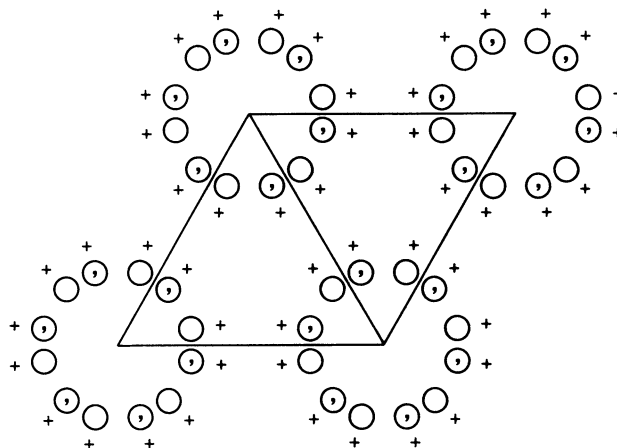
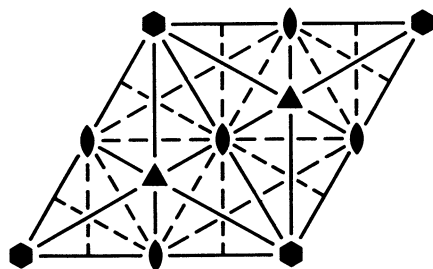
$6mm$

Hexagonal

No. 183

$P6mm$

Patterson symmetry $P6/mmm$



Origin on $6mm$

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{3}$; $0 \leq z \leq 1$; $x \leq (1+y)/2$; $y \leq x/2$
 Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$
 $0, 0, 1$ $\frac{1}{2}, 0, 1$ $\frac{2}{3}, \frac{1}{3}, 1$

Symmetry operations

- | | | |
|-------------------------|---------------------|---------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) 2 $0, 0, z$ | (5) 6^- $0, 0, z$ | (6) 6^+ $0, 0, z$ |
| (7) m x, \bar{x}, z | (8) m $x, 2x, z$ | (9) m $2x, x, z$ |
| (10) m x, x, z | (11) m $x, 0, z$ | (12) m $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions
								General:
								no conditions
12 f 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$					
	(4) \bar{x}, \bar{y}, z	(5) $y, \bar{x} + y, z$	(6) $x - y, x, z$					
	(7) \bar{y}, \bar{x}, z	(8) $\bar{x} + y, y, z$	(9) $x, x - y, z$					
	(10) y, x, z	(11) $x - y, \bar{y}, z$	(12) $\bar{x}, \bar{x} + y, z$					
								Special: no extra conditions
6 e $.m.$	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	\bar{x}, x, z	$\bar{x}, 2\bar{x}, z$	$2x, x, z$		
6 d $.m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$\bar{x}, 0, z$	$0, \bar{x}, z$	x, x, z		
3 c $2mm$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z$					
2 b $3m.$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$						
1 a $6mm$	$0, 0, z$							

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P611$ ($P6, 168$)	1; 2; 3; 4; 5; 6
	[2] $P31m$ (157)	1; 2; 3; 10; 11; 12
	[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9
	{ [3] $P2mm$ ($Cmm2, 35$)	1; 4; 7; 10
	{ [3] $P2mm$ ($Cmm2, 35$)	1; 4; 8; 11
	{ [3] $P2mm$ ($Cmm2, 35$)	1; 4; 9; 12

IIa none

IIb [2] $P6_3mc$ ($\mathbf{c}' = 2\mathbf{c}$) (186); [2] $P6_3cm$ ($\mathbf{c}' = 2\mathbf{c}$) (185); [2] $P6cc$ ($\mathbf{c}' = 2\mathbf{c}$) (184)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6mm$ ($\mathbf{c}' = 2\mathbf{c}$) (183); [3] $H6mm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6mm, 183$)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191)

II none

$P6cc$

C_{6v}^2

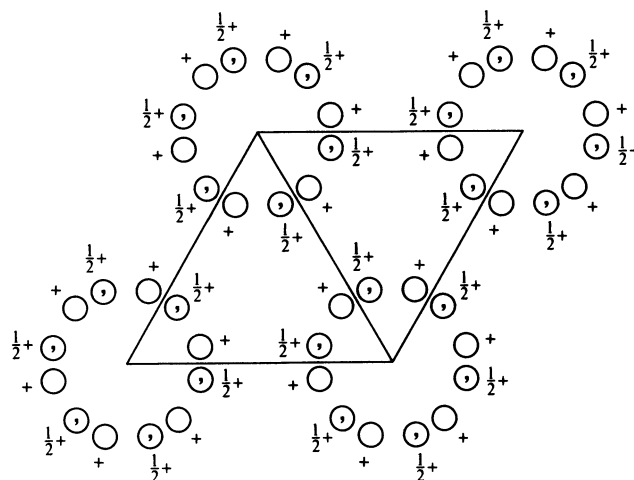
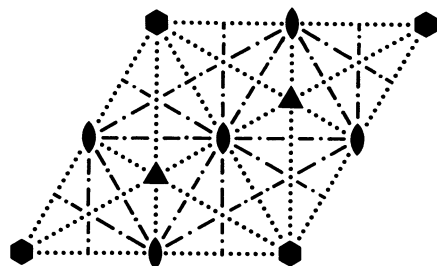
$6mm$

Hexagonal

No. 184

$P6cc$

Patterson symmetry $P6/mmm$



Origin on $6cc$

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|-------------------------|---------------------|---------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) 2 $0, 0, z$ | (5) 6^- $0, 0, z$ | (6) 6^+ $0, 0, z$ |
| (7) c x, \bar{x}, z | (8) c $x, 2x, z$ | (9) c $2x, x, z$ |
| (10) c x, x, z | (11) c $x, 0, z$ | (12) c $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>d</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) \bar{x}, \bar{y}, z (5) $y, \bar{x} + y, z$ (6) $x - y, x, z$ (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (8) $\bar{x} + y, y, z + \frac{1}{2}$ (9) $x, x - y, z + \frac{1}{2}$ (10) $y, x, z + \frac{1}{2}$ (11) $x - y, \bar{y}, z + \frac{1}{2}$ (12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$: $l = 2n$ $h\bar{h}0l$: $l = 2n$ $000l$: $l = 2n$ Special: as above, plus
6 <i>c</i> 2..	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkil$: $l = 2n$
4 <i>b</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z$ $\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$hkil$: $l = 2n$
2 <i>a</i> 6..	$0, 0, z$ $0, 0, z + \frac{1}{2}$	$hkil$: $l = 2n$

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, 0, 0$

Along [210] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P611$ ($P6$, 168)	1; 2; 3; 4; 5; 6
	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9
	{ [3] $P2cc$ ($Ccc2$, 37)	1; 4; 7; 10
	{ [3] $P2cc$ ($Ccc2$, 37)	1; 4; 8; 11
	{ [3] $P2cc$ ($Ccc2$, 37)	1; 4; 9; 12

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P6cc$ ($\mathbf{c}' = 3\mathbf{c}$) (184); [3] $H6cc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6cc$, 184)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192)

II [2] $P6mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (183)

$P6_3cm$

C_{6v}^3

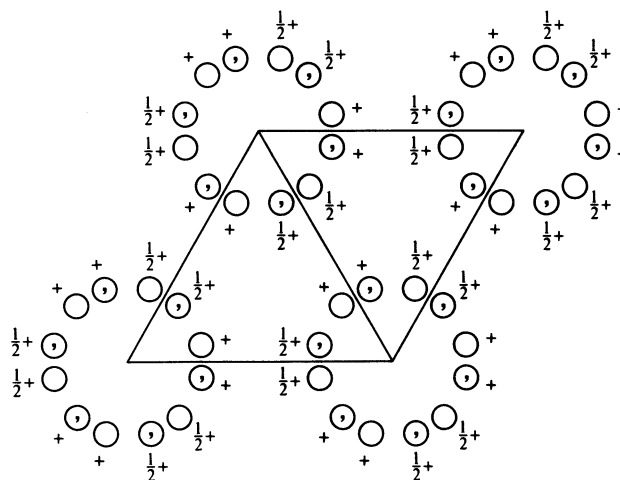
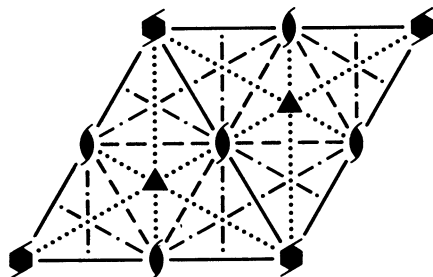
$6mm$

Hexagonal

No. 185

$P6_3cm$

Patterson symmetry $P6/mmm$



Origin on $31m$ on 6_3cm

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|------------------------------------|--------------------------------------|--------------------------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2}) 0, 0, z$ | (5) $6^-(0, 0, \frac{1}{2}) 0, 0, z$ | (6) $6^+(0, 0, \frac{1}{2}) 0, 0, z$ |
| (7) $c x, \bar{x}, z$ | (8) $c x, 2x, z$ | (9) $c 2x, x, z$ |
| (10) $m x, x, z$ | (11) $m x, 0, z$ | (12) $m 0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
							General:
12 <i>d</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$				$h\bar{h}0l : l = 2n$
	(4) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(5) $y, \bar{x} + y, z + \frac{1}{2}$	(6) $x - y, x, z + \frac{1}{2}$				$000l : l = 2n$
	(7) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(8) $\bar{x} + y, y, z + \frac{1}{2}$	(9) $x, x - y, z + \frac{1}{2}$				
	(10) y, x, z	(11) $x - y, \bar{y}, z$	(12) $\bar{x}, \bar{x} + y, z$				
							Special: as above, plus
6 <i>c</i> $. . m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$\bar{x}, 0, z + \frac{1}{2}$	$0, \bar{x}, z + \frac{1}{2}$	$x, x, z + \frac{1}{2}$	no extra conditions
4 <i>b</i> $3 . .$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, z$			$hkil : l = 2n$
2 <i>a</i> $3 . m$	$0, 0, z$	$0, 0, z + \frac{1}{2}$					$hkil : l = 2n$

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p1m1$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [210] $p1g1$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P6_311$ ($P6_3, 173$)	1; 2; 3; 4; 5; 6
	[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9
	[2] $P31m$ (157)	1; 2; 3; 10; 11; 12
	{ [3] $P2_1cm$ ($Cmc2_1, 36$)	1; 4; 7; 10
	{ [3] $P2_1cm$ ($Cmc2_1, 36$)	1; 4; 8; 11
	{ [3] $P2_1cm$ ($Cmc2_1, 36$)	1; 4; 9; 12

IIa none

IIIb [3] $H6_3cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3mc, 186$)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3cm$ ($\mathbf{c}' = 3\mathbf{c}$) (185); [4] $P6_3cm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (185)

Minimal non-isomorphic supergroups

I [2] $P6_3/mcm$ (193)

II [3] $H6_3cm$ ($P6_3mc, 186$); [2] $P6mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (183)

$P6_3mc$

C_{6v}^4

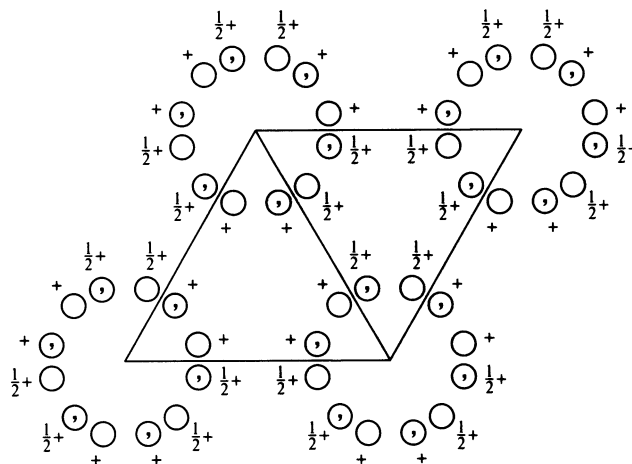
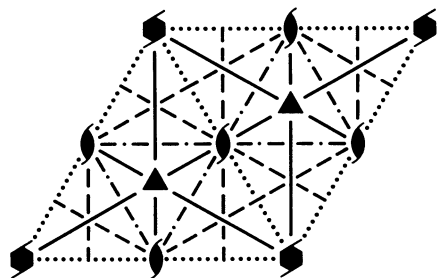
$6mm$

Hexagonal

No. 186

$P6_3mc$

Patterson symmetry $P6/mmm$



Origin on $3m1$ on 6_3mc

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{3}$; $0 \leq z \leq 1$; $x \leq (1+y)/2$; $y \leq x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$
 $0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$

Symmetry operations

- | | | |
|--------------------------------|----------------------------------|----------------------------------|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) $2(0,0,\frac{1}{2}) 0,0,z$ | (5) $6^-(0,0,\frac{1}{2}) 0,0,z$ | (6) $6^+(0,0,\frac{1}{2}) 0,0,z$ |
| (7) $m x,\bar{x},z$ | (8) $m x,2x,z$ | (9) $m 2x,x,z$ |
| (10) $c x,x,z$ | (11) $c x,0,z$ | (12) $c 0,y,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
							General:
12 <i>d</i> 1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$				$hh\bar{2}hl$: $l = 2n$
	(4) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(5) $y, \bar{x} + y, z + \frac{1}{2}$	(6) $x - y, x, z + \frac{1}{2}$				$000l$: $l = 2n$
	(7) \bar{y}, \bar{x}, z	(8) $\bar{x} + y, y, z$	(9) $x, x - y, z$				
	(10) $y, x, z + \frac{1}{2}$	(11) $x - y, \bar{y}, z + \frac{1}{2}$	(12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$				
							Special: as above, plus
6 <i>c</i> . <i>m</i> .	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	$\bar{x}, x, z + \frac{1}{2}$	$\bar{x}, 2\bar{x}, z + \frac{1}{2}$	$2x, x, z + \frac{1}{2}$	no extra conditions
2 <i>b</i> 3 <i>m</i> .	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$					$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>a</i> 3 <i>m</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$					$hkil$: $l = 2n$

Symmetry of special projections

Along [001] $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p1g1$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P6_311$ ($P6_3, 173$)	1; 2; 3; 4; 5; 6
	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9
	{ [3] $P2_1mc$ ($Cmc2_1, 36$)	1; 4; 7; 10
		1; 4; 8; 11
		1; 4; 9; 12

IIa none

IIb [3] $H6_3mc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3cm, 185$)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3mc$ ($\mathbf{c}' = 3\mathbf{c}$) (186); [4] $P6_3mc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (186)

Minimal non-isomorphic supergroups

I [2] $P6_3/mmc$ (194)

II [3] $H6_3mc$ ($P6_3cm, 185$); [2] $P6mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (183)

$P\bar{6}m2$

D_{3h}^1

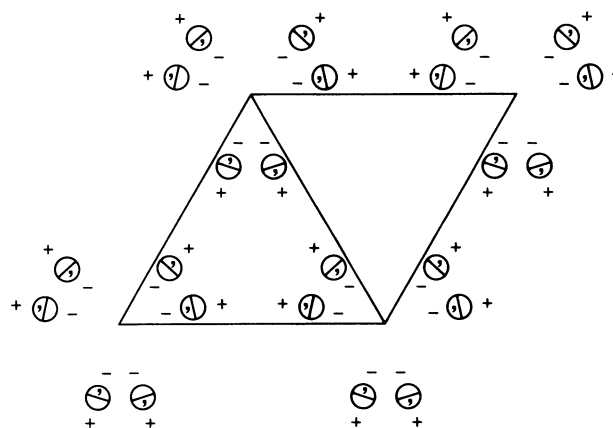
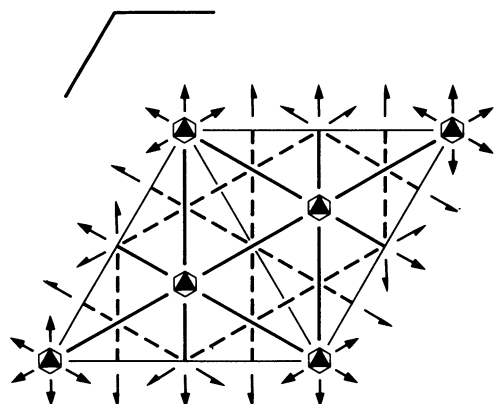
$\bar{6}m2$

Hexagonal

No. 187

$P\bar{6}m2$

Patterson symmetry $P6/mmm$



Origin at $\bar{6}m2$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{2}; x \leq 2y; y \leq \min(1-x, 2x)$

Vertices $0, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
 $0, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$

Symmetry operations

- | | | |
|--------------------------|------------------------------------|------------------------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) m $x, y, 0$ | (5) $\bar{6}^-$ $0, 0, z; 0, 0, 0$ | (6) $\bar{6}^+$ $0, 0, z; 0, 0, 0$ |
| (7) m x, \bar{x}, z | (8) m $x, 2x, z$ | (9) m $2x, x, z$ |
| (10) 2 $x, \bar{x}, 0$ | (11) 2 $x, 2x, 0$ | (12) 2 $2x, x, 0$ |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{6}11$ ($P\bar{6}$, 174) 1; 2; 3; 4; 5; 6
 [2] $P3m1$ (156) 1; 2; 3; 7; 8; 9
 [2] $P312$ (149) 1; 2; 3; 10; 11; 12
 { [3] $Pmm2$ ($Amm2$, 38) 1; 4; 7; 10
 [3] $Pmm2$ ($Amm2$, 38) 1; 4; 8; 11
 [3] $Pmm2$ ($Amm2$, 38) 1; 4; 9; 12

IIa none

IIb [2] $P\bar{6}c2$ ($c' = 2c$) (188); [3] $H\bar{6}m2$ ($a' = 3a, b' = 3b$) ($P\bar{6}2m$, 189)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{6}m2$ ($c' = 2c$) (187); [4] $P\bar{6}m2$ ($a' = 2a, b' = 2b$) (187)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II [3] $H\bar{6}m2$ ($P\bar{6}2m$, 189)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

12	<i>o</i>	1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$
			(4) x, y, \bar{z}	(5) $\bar{y}, x - y, \bar{z}$	(6) $\bar{x} + y, \bar{x}, \bar{z}$
			(7) \bar{y}, \bar{x}, z	(8) $\bar{x} + y, y, z$	(9) $x, x - y, z$
			(10) $\bar{y}, \bar{x}, \bar{z}$	(11) $\bar{x} + y, y, \bar{z}$	(12) $x, x - y, \bar{z}$

General:

no conditions

Special: no extra conditions

6	<i>n</i>	$.m.$	x, \bar{x}, z	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	x, \bar{x}, \bar{z}	$x, 2x, \bar{z}$	$2\bar{x}, \bar{x}, \bar{z}$
6	<i>m</i>	$m..$	$x, y, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$	$\bar{y}, \bar{x}, \frac{1}{2}$	$\bar{x} + y, y, \frac{1}{2}$	$x, x - y, \frac{1}{2}$
6	<i>l</i>	$m..$	$x, y, 0$	$\bar{y}, x - y, 0$	$\bar{x} + y, \bar{x}, 0$	$\bar{y}, \bar{x}, 0$	$\bar{x} + y, y, 0$	$x, x - y, 0$
3	<i>k</i>	$mm2$	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$			
3	<i>j</i>	$mm2$	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$			
2	<i>i</i>	$3m.$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$				
2	<i>h</i>	$3m.$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$				
2	<i>g</i>	$3m.$	$0, 0, z$	$0, 0, \bar{z}$				
1	<i>f</i>	$\bar{6}m2$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$					
1	<i>e</i>	$\bar{6}m2$	$\frac{2}{3}, \frac{1}{3}, 0$					
1	<i>d</i>	$\bar{6}m2$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$					
1	<i>c</i>	$\bar{6}m2$	$\frac{1}{3}, \frac{2}{3}, 0$					
1	<i>b</i>	$\bar{6}m2$	$0, 0, \frac{1}{2}$					
1	<i>a</i>	$\bar{6}m2$	$0, 0, 0$					

Symmetry of special projectionsAlong [001] $p3m1$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along [100] $p11m$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$ Along [210] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

(Continued on preceding page)

$P\bar{6}c2$

D_{3h}^2

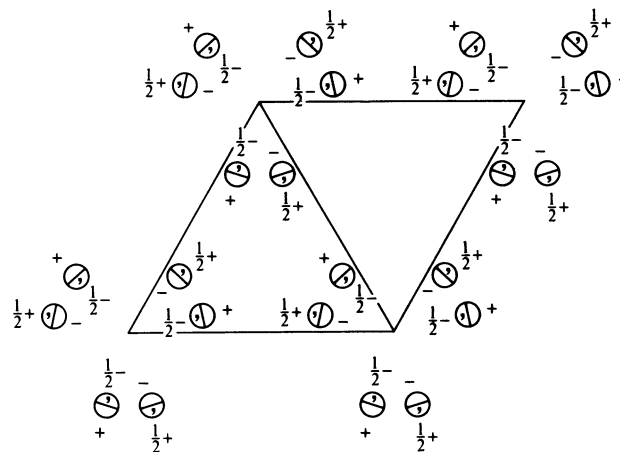
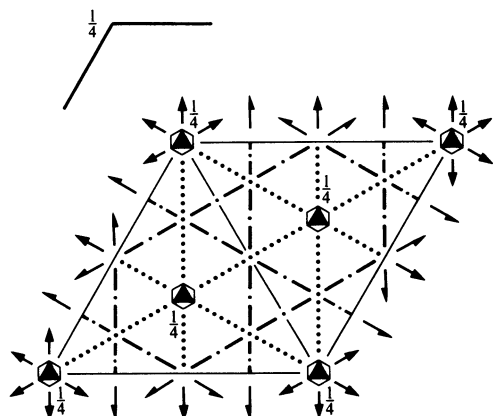
$\bar{6}m2$

Hexagonal

No. 188

$P\bar{6}c2$

Patterson symmetry $P6/mmm$



Origin at $3c2$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{4}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$ $0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|-----------------------------|--|--|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) m $x, y, \frac{1}{4}$ | (5) $\bar{6}^-$ $0, 0, z; 0, 0, \frac{1}{4}$ | (6) $\bar{6}^+$ $0, 0, z; 0, 0, \frac{1}{4}$ |
| (7) c x, \bar{x}, z | (8) c $x, 2x, z$ | (9) c $2x, x, z$ |
| (10) 2 $x, \bar{x}, 0$ | (11) 2 $x, 2x, 0$ | (12) 2 $2x, x, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>l</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $x, y, \bar{z} + \frac{1}{2}$ (5) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$ (6) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$ (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (8) $\bar{x} + y, y, z + \frac{1}{2}$ (9) $x, x - y, z + \frac{1}{2}$ (10) $\bar{y}, \bar{x}, \bar{z}$ (11) $\bar{x} + y, y, \bar{z}$ (12) $x, x - y, \bar{z}$	General: $h\bar{h}0l : l = 2n$ $000l : l = 2n$
		Special: as above, plus
6 <i>k</i> $m..$	$x, y, \frac{1}{4}$ $\bar{y}, x - y, \frac{1}{4}$ $\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{y}, \bar{x}, \frac{3}{4}$ $\bar{x} + y, y, \frac{3}{4}$ $x, x - y, \frac{3}{4}$	no extra conditions
6 <i>j</i> $..2$	$x, \bar{x}, 0$ $x, 2x, 0$ $2\bar{x}, \bar{x}, 0$ $x, \bar{x}, \frac{1}{2}$ $x, 2x, \frac{1}{2}$ $2\bar{x}, \bar{x}, \frac{1}{2}$	$hkil : l = 2n$
4 <i>i</i> $3..$	$\frac{2}{3}, \frac{1}{3}, z$ $\frac{2}{3}, \frac{1}{3}, \bar{z} + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$	$hkil : l = 2n$
4 <i>h</i> $3..$	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \bar{z}$	$hkil : l = 2n$
4 <i>g</i> $3..$	$0, 0, z$ $0, 0, \bar{z} + \frac{1}{2}$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z}$	$hkil : l = 2n$
2 <i>f</i> $\bar{6}..$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$hkil : l = 2n$
2 <i>e</i> 3.2	$\frac{2}{3}, \frac{1}{3}, 0$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$	$hkil : l = 2n$
2 <i>d</i> $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$	$hkil : l = 2n$
2 <i>c</i> 3.2	$\frac{1}{3}, \frac{2}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$hkil : l = 2n$
2 <i>b</i> $\bar{6}..$	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkil : l = 2n$
2 <i>a</i> 3.2	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkil : l = 2n$

Symmetry of special projections

Along [001] $p3m1$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p11m$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}11$ ($P\bar{6}$, 174)	1; 2; 3; 4; 5; 6
	[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9
	[2] $P312$ (149)	1; 2; 3; 10; 11; 12
	{ [3] $Pmc2$ ($Ama2$, 40)	1; 4; 7; 10
	{ [3] $Pmc2$ ($Ama2$, 40)	1; 4; 8; 11
	{ [3] $Pmc2$ ($Ama2$, 40)	1; 4; 9; 12

IIa none

IIb [3] $H\bar{6}c2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{6}2c$, 190)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{6}c2$ ($\mathbf{c}' = 3\mathbf{c}$) (188); [4] $P\bar{6}c2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (188)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

II [3] $H\bar{6}c2$ ($P\bar{6}2c$, 190); [2] $P\bar{6}m2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (187)

$P\bar{6}2m$

D_{3h}^3

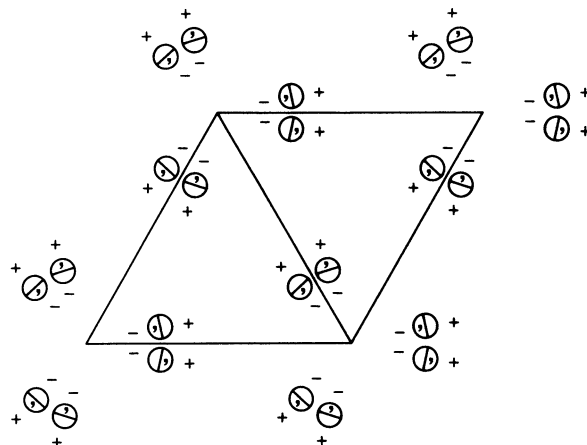
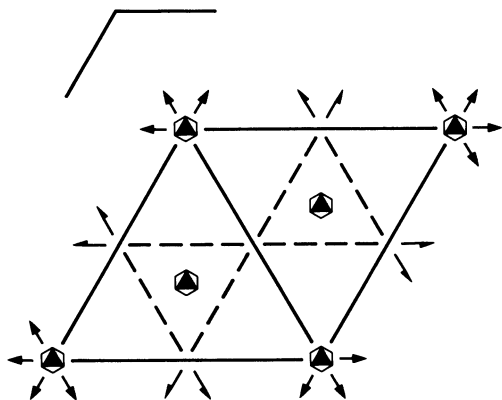
$\bar{6}2m$

Hexagonal

No. 189

$P\bar{6}2m$

Patterson symmetry $P6/mmm$



Origin at $\bar{6}2m$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq \min(1-x, x)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | |
|--------------------|------------------------------------|------------------------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) m $x, y, 0$ | (5) $\bar{6}^-$ $0, 0, z; 0, 0, 0$ | (6) $\bar{6}^+$ $0, 0, z; 0, 0, 0$ |
| (7) 2 $x, x, 0$ | (8) 2 $x, 0, 0$ | (9) 2 $0, y, 0$ |
| (10) m x, x, z | (11) m $x, 0, z$ | (12) m $0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions	
						General:	
12	l 1	(1) x, y, z (4) x, y, \bar{z} (7) y, x, \bar{z} (10) y, x, z	(2) $\bar{y}, x - y, z$ (5) $\bar{y}, x - y, \bar{z}$ (8) $x - y, \bar{y}, \bar{z}$ (11) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x} + y, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $\bar{x}, \bar{x} + y, z$		no conditions	
						Special: no extra conditions	
6	k $m..$	$x, y, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$	$y, x, \frac{1}{2}$	$x - y, \bar{y}, \frac{1}{2}$	$\bar{x}, \bar{x} + y, \frac{1}{2}$
6	j $m..$	$x, y, 0$	$\bar{y}, x - y, 0$	$\bar{x} + y, \bar{x}, 0$	$y, x, 0$	$x - y, \bar{y}, 0$	$\bar{x}, \bar{x} + y, 0$
6	i $..m$	$x, 0, z$	$0, x, z$	\bar{x}, \bar{x}, z	$x, 0, \bar{z}$	$0, x, \bar{z}$	$\bar{x}, \bar{x}, \bar{z}$
4	h $3..$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z$		
3	g $m2m$	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$			
3	f $m2m$	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$			
2	e $3.m$	$0, 0, z$	$0, 0, \bar{z}$				
2	d $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$				
2	c $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$				
1	b $\bar{6}2m$	$0, 0, \frac{1}{2}$					
1	a $\bar{6}2m$	$0, 0, 0$					

Symmetry of special projections

Along [001] $p31m$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}11$ ($P\bar{6}$, 174)	1; 2; 3; 4; 5; 6
	[2] $P31m$ (157)	1; 2; 3; 10; 11; 12
	[2] $P321$ (150)	1; 2; 3; 7; 8; 9
	{ [3] $Pm2m$ ($Amm2$, 38)	1; 4; 7; 10
	{ [3] $Pm2m$ ($Amm2$, 38)	1; 4; 8; 11
	{ [3] $Pm2m$ ($Amm2$, 38)	1; 4; 9; 12

IIa none

IIb [2] $P\bar{6}2c$ ($\mathbf{c}' = 2\mathbf{c}$) (190); [3] $H\bar{6}2m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{6}m2$, 187)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{6}2m$ ($\mathbf{c}' = 2\mathbf{c}$) (189); [4] $P\bar{6}2m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (189)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)

II [3] $H\bar{6}2m$ ($P\bar{6}m2$, 187)

$P\bar{6}2c$

D_{3h}^4

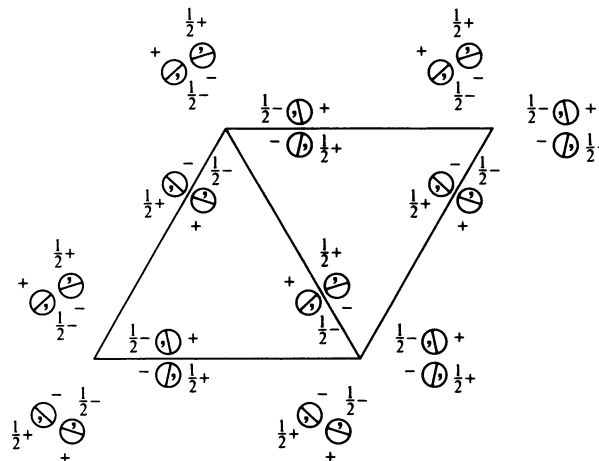
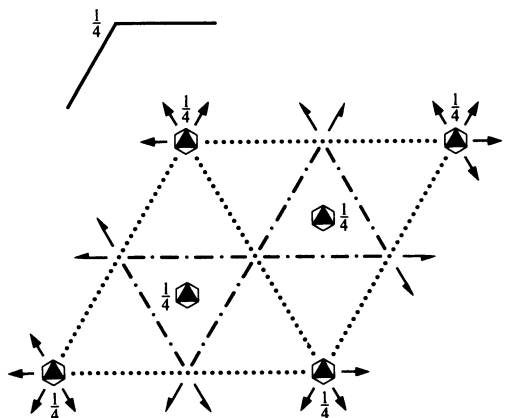
$\bar{6}2m$

Hexagonal

No. 190

$P\bar{6}2c$

Patterson symmetry $P6/mmm$



Origin at $32c$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{4}; x \leq (1+y)/2; y \leq \min(1-x, (1+x)/2)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{2}{3}, \frac{1}{3}, 0 \quad \frac{1}{3}, \frac{2}{3}, 0 \quad 0, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4} \quad \frac{1}{2}, 0, \frac{1}{4} \quad \frac{2}{3}, \frac{1}{3}, \frac{1}{4} \quad \frac{1}{3}, \frac{2}{3}, \frac{1}{4} \quad 0, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|---------------------------|--|--|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $m x, y, \frac{1}{4}$ | (5) $\bar{6}^- 0, 0, z; 0, 0, \frac{1}{4}$ | (6) $\bar{6}^+ 0, 0, z; 0, 0, \frac{1}{4}$ |
| (7) $2 x, x, 0$ | (8) $2 x, 0, 0$ | (9) $2 0, y, 0$ |
| (10) $c x, x, z$ | (11) $c x, 0, z$ | (12) $c 0, y, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions			
12 <i>i</i> 1	(1) x, y, z (4) $x, y, \bar{z} + \frac{1}{2}$ (7) y, x, \bar{z} (10) $y, x, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$ (8) $x - y, \bar{y}, \bar{z}$ (11) $x - y, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$: $l = 2n$ $000l$: $l = 2n$ Special: as above, plus			
6 <i>h</i> $m..$	$x, y, \frac{1}{4}$	$\bar{y}, x - y, \frac{1}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$	$y, x, \frac{3}{4}$	$x - y, \bar{y}, \frac{3}{4}$	$\bar{x}, \bar{x} + y, \frac{3}{4}$	no extra conditions
6 <i>g</i> $.2.$	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$hkil$: $l = 2n$
4 <i>f</i> $3..$	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$			$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> $3..$	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$			$hkil$: $l = 2n$
2 <i>d</i> $\bar{6}..$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$					$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> $\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$					$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>b</i> $\bar{6}..$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					$hkil$: $l = 2n$
2 <i>a</i> $32.$	$0, 0, 0$	$0, 0, \frac{1}{2}$					$hkil$: $l = 2n$

Symmetry of special projections

Along $[001]$ $p31m$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[210]$ $p11m$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}11$ ($P\bar{6}$, 174)	1; 2; 3; 4; 5; 6
	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P321$ (150)	1; 2; 3; 7; 8; 9
	{ [3] $Pm2c$ ($Ama2$, 40)	1; 4; 7; 10
	{ [3] $Pm2c$ ($Ama2$, 40)	1; 4; 8; 11
	{ [3] $Pm2c$ ($Ama2$, 40)	1; 4; 9; 12

IIa none

IIb [3] $H\bar{6}2c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{6}c2$, 188)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{6}2c$ ($\mathbf{c}' = 3\mathbf{c}$) (190); [4] $P\bar{6}2c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (190)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

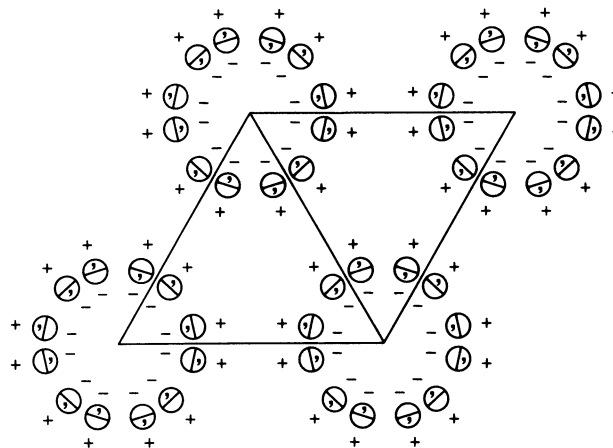
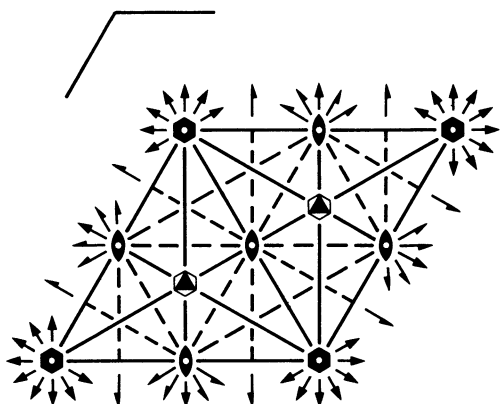
II [3] $H\bar{6}2c$ ($P\bar{6}c2$, 188); [2] $P\bar{6}2m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (189)

$P6/mmm$
 D_{6h}^1
 $6/mmm$

Hexagonal

No. 191

 $P 6/m 2/m 2/m$

 Patterson symmetry $P6/mmm$

Origin at centre ($6/mmm$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{3}; 0 \leq z \leq \frac{1}{2}; x \leq (1+y)/2; y \leq x/2$
Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0$
 $0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2}$
Symmetry operations

- | | | |
|----------------------|-------------------------------|-------------------------------|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) 2 $0,0,z$ | (5) $6^- 0,0,z$ | (6) $6^+ 0,0,z$ |
| (7) 2 $x,x,0$ | (8) 2 $x,0,0$ | (9) 2 $0,y,0$ |
| (10) 2 $x,\bar{x},0$ | (11) 2 $x,2x,0$ | (12) 2 $2x,x,0$ |
| (13) $\bar{1} 0,0,0$ | (14) $\bar{3}^+ 0,0,z; 0,0,0$ | (15) $\bar{3}^- 0,0,z; 0,0,0$ |
| (16) $m x,y,0$ | (17) $\bar{6}^- 0,0,z; 0,0,0$ | (18) $\bar{6}^+ 0,0,z; 0,0,0$ |
| (19) $m x,\bar{x},z$ | (20) $m x,2x,z$ | (21) $m 2x,x,z$ |
| (22) $m x,x,z$ | (23) $m x,0,z$ | (24) $m 0,y,z$ |

Maximal non-isomorphic subgroups

- | | | |
|----------|------------------------------|---|
| I | [2] $P\bar{6}2m$ (189) | 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24 |
| | [2] $P\bar{6}m2$ (187) | 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21 |
| | [2] $P6mm$ (183) | 1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24 |
| | [2] $P622$ (177) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12 |
| | [2] $P6/m11$ ($P6/m$, 175) | 1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18 |
| | [2] $P\bar{3}m1$ (164) | 1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21 |
| | [2] $P\bar{3}1m$ (162) | 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24 |
| | { [3] $Pmmm$ ($Cmmm$, 65) | 1; 4; 7; 10; 13; 16; 19; 22 |
| | { [3] $Pmmm$ ($Cmmm$, 65) | 1; 4; 8; 11; 13; 16; 20; 23 |
| | { [3] $Pmmm$ ($Cmmm$, 65) | 1; 4; 9; 12; 13; 16; 21; 24 |

IIa none

IIb [2] $P6_3/mmc$ ($c' = 2c$) (194); [2] $P6_3/mcm$ ($c' = 2c$) (193); [2] $P6/mcc$ ($c' = 2c$) (192)

Maximal isomorphic subgroups of lowest index
IIc [2] $P6/mmm$ ($c' = 2c$) (191); [3] $H6/mmm$ ($a' = 3a, b' = 3b$) ($P6/mmm$, 191)

Minimal non-isomorphic supergroups
I none

II none

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
								General:
24	<i>r</i> 1	(1) x, y, z (4) \bar{x}, \bar{y}, z (7) y, x, \bar{z} (10) $\bar{y}, \bar{x}, \bar{z}$ (13) $\bar{x}, \bar{y}, \bar{z}$ (16) x, y, \bar{z} (19) \bar{y}, \bar{x}, z (22) y, x, z	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z$ (8) $x - y, \bar{y}, \bar{z}$ (11) $\bar{x} + y, y, \bar{z}$ (14) $y, \bar{x} + y, \bar{z}$ (17) $\bar{y}, x - y, \bar{z}$ (20) $\bar{x} + y, y, z$ (23) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $x, x - y, \bar{z}$ (15) $x - y, x, \bar{z}$ (18) $\bar{x} + y, \bar{x}, \bar{z}$ (21) $x, x - y, z$ (24) $\bar{x}, \bar{x} + y, z$				no conditions
								Special: no extra conditions
12	<i>q</i> <i>m</i> . .	$x, y, \frac{1}{2}$ $y, x, \frac{1}{2}$	$\bar{y}, x - y, \frac{1}{2}$ $x - y, \bar{y}, \frac{1}{2}$	$\bar{x} + y, \bar{x}, \frac{1}{2}$ $\bar{x}, \bar{x} + y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	$y, \bar{x} + y, \frac{1}{2}$ $\bar{x} + y, y, \frac{1}{2}$	$x - y, x, \frac{1}{2}$ $x, x - y, \frac{1}{2}$	
12	<i>p</i> <i>m</i> . .	$x, y, 0$ $y, x, 0$	$\bar{y}, x - y, 0$ $x - y, \bar{y}, 0$	$\bar{x} + y, \bar{x}, 0$ $\bar{x}, \bar{x} + y, 0$	$\bar{x}, \bar{y}, 0$ $\bar{y}, \bar{x}, 0$	$y, \bar{x} + y, 0$ $\bar{x} + y, y, 0$	$x - y, x, 0$ $x, x - y, 0$	
12	<i>o</i> . <i>m</i> .	$x, 2x, z$ $2x, x, \bar{z}$	$2\bar{x}, \bar{x}, z$ $\bar{x}, 2\bar{x}, \bar{z}$	x, \bar{x}, z \bar{x}, x, \bar{z}	$\bar{x}, 2\bar{x}, z$ $2\bar{x}, \bar{x}, \bar{z}$	$2x, x, z$ $x, 2x, \bar{z}$	\bar{x}, x, z x, \bar{x}, \bar{z}	
12	<i>n</i> . . <i>m</i>	$x, 0, z$ $0, x, \bar{z}$	$0, x, z$ $x, 0, \bar{z}$	\bar{x}, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	$\bar{x}, 0, z$ $0, \bar{x}, \bar{z}$	$0, \bar{x}, z$ $\bar{x}, 0, \bar{z}$	x, x, z x, x, \bar{z}	
6	<i>m</i> <i>m</i> <i>m</i> 2	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	
6	<i>l</i> <i>m</i> <i>m</i> 2	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$x, \bar{x}, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$	$\bar{x}, x, 0$	
6	<i>k</i> <i>m</i> 2 <i>m</i>	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$	
6	<i>j</i> <i>m</i> 2 <i>m</i>	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$	
6	<i>i</i> 2 <i>m</i> <i>m</i>	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	
4	<i>h</i> 3 <i>m</i> .	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$			
3	<i>g</i> <i>m</i> <i>m</i> <i>m</i>	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				
3	<i>f</i> <i>m</i> <i>m</i> <i>m</i>	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$				
2	<i>e</i> 6 <i>m</i> <i>m</i>	$0, 0, z$	$0, 0, \bar{z}$					
2	<i>d</i> $\bar{6}$ <i>m</i> 2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$					
2	<i>c</i> $\bar{6}$ <i>m</i> 2	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$					
1	<i>b</i> 6/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, \frac{1}{2}$						
1	<i>a</i> 6/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, 0$						

Symmetry of special projections

Along [001] *p6mm*
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] *p2mm*
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [210] *p2mm*
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

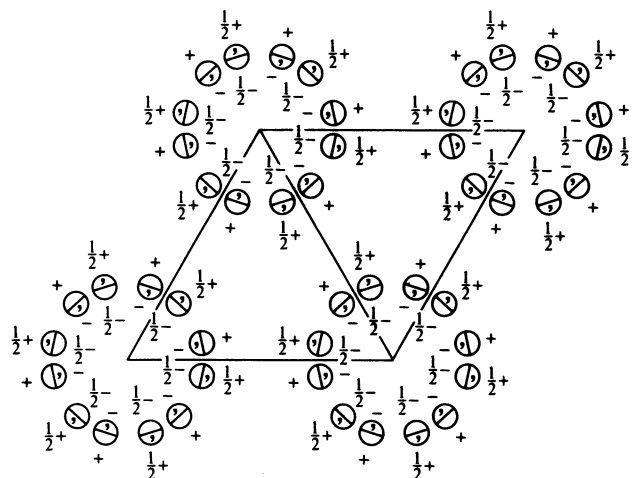
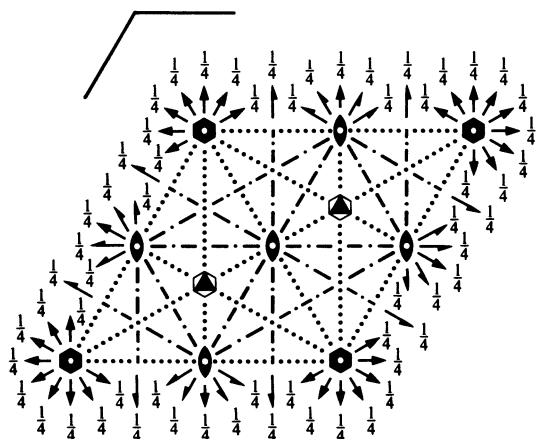
(Continued on preceding page)

$P6/mcc$
 D_{6h}^2
 $6/mmm$

Hexagonal

No. 192

 $P 6/m 2/c 2/c$

 Patterson symmetry $P6/mmm$

Origin at centre ($6/m$) at $6/mcc$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{1}{3}; 0 \leq z \leq \frac{1}{4}; x \leq (1+y)/2; y \leq \min(1-x, x)$
Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

- | | | |
|----------------------------------|-----------------------------------|-----------------------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) 2 $0, 0, z$ | (5) $6^- 0, 0, z$ | (6) $6^+ 0, 0, z$ |
| (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, 0, \frac{1}{4}$ | (9) 2 $0, y, \frac{1}{4}$ |
| (10) 2 $x, \bar{x}, \frac{1}{4}$ | (11) 2 $x, 2x, \frac{1}{4}$ | (12) 2 $2x, x, \frac{1}{4}$ |
| (13) $\bar{1} 0, 0, 0$ | (14) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (15) $\bar{3}^- 0, 0, z; 0, 0, 0$ |
| (16) $m x, y, 0$ | (17) $\bar{6}^- 0, 0, z; 0, 0, 0$ | (18) $\bar{6}^+ 0, 0, z; 0, 0, 0$ |
| (19) $c x, \bar{x}, z$ | (20) $c x, 2x, z$ | (21) $c 2x, x, z$ |
| (22) $c x, x, z$ | (23) $c x, 0, z$ | (24) $c 0, y, z$ |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{6}2c$ (190) 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
 [2] $P\bar{6}c2$ (188) 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
 [2] $P6cc$ (184) 1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
 [2] $P622$ (177) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
 [2] $P6/m11$ ($P6/m$, 175) 1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
 [2] $P\bar{3}c1$ (165) 1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
 [2] $P\bar{3}1c$ (163) 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
 { [3] $Pmcc$ ($Cccm$, 66) 1; 4; 7; 10; 13; 16; 19; 22
 [3] $Pmcc$ ($Cccm$, 66) 1; 4; 8; 11; 13; 16; 20; 23
 [3] $Pmcc$ ($Cccm$, 66) 1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

- IIc** [3] $P6/mcc$ ($c' = 3c$) (192); [3] $H6/mcc$ ($a' = 3a, b' = 3b$) ($P6/mcc$, 192)

Minimal non-isomorphic supergroups
I none

- II** [2] $P6/mmm$ ($c' = \frac{1}{2}c$) (191)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions
24 <i>m</i> 1	(1) x, y, z (4) \bar{x}, \bar{y}, z (7) $y, x, \bar{z} + \frac{1}{2}$ (10) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (13) $\bar{x}, \bar{y}, \bar{z}$ (16) x, y, \bar{z} (19) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (22) $y, x, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z$ (8) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$ (11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$ (14) $y, \bar{x} + y, \bar{z}$ (17) $\bar{y}, x - y, \bar{z}$ (20) $\bar{x} + y, y, z + \frac{1}{2}$ (23) $x - y, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z$ (9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$ (12) $x, x - y, \bar{z} + \frac{1}{2}$ (15) $x - y, x, \bar{z}$ (18) $\bar{x} + y, \bar{x}, \bar{z}$ (21) $x, x - y, z + \frac{1}{2}$ (24) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$					General: $hh\bar{2}hl$: $l = 2n$ $h\bar{h}0l$: $l = 2n$ $000l$: $l = 2n$
12 <i>l</i> <i>m</i> . .	$x, y, 0$ $y, x, \frac{1}{2}$	$\bar{y}, x - y, 0$ $x - y, \bar{y}, \frac{1}{2}$	$\bar{x} + y, \bar{x}, 0$ $\bar{x}, \bar{x} + y, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $\bar{y}, \bar{x}, \frac{1}{2}$	$y, \bar{x} + y, 0$ $\bar{x} + y, y, \frac{1}{2}$	$x - y, x, 0$ $x, x - y, \frac{1}{2}$	Special: as above, plus no extra conditions	
12 <i>k</i> . . 2	$x, 2x, \frac{1}{4}$ $\bar{x}, 2\bar{x}, \frac{3}{4}$	$2\bar{x}, \bar{x}, \frac{1}{4}$ $2x, x, \frac{3}{4}$	$x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$	$\bar{x}, 2\bar{x}, \frac{1}{4}$ $x, 2x, \frac{3}{4}$	$2x, x, \frac{1}{4}$ $2\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, x, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$	$hkil$: $l = 2n$	
12 <i>j</i> . 2 .	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$0, x, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x, x, \frac{3}{4}$	$\bar{x}, 0, \frac{1}{4}$ $x, 0, \frac{3}{4}$	$0, \bar{x}, \frac{1}{4}$ $0, x, \frac{3}{4}$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$hkil$: $l = 2n$	
12 <i>i</i> 2 . .	$\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkil$: $l = 2n$	
8 <i>h</i> 3 . .	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z$ $\frac{1}{3}, \frac{2}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, \bar{z} + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$	$\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$			$hkil$: $l = 2n$	
6 <i>g</i> 2/ <i>m</i> . .	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil$: $l = 2n$	
6 <i>f</i> 222	$\frac{1}{2}, 0, \frac{1}{4}$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkil$: $l = 2n$	
4 <i>e</i> 6 . .	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$			$hkil$: $l = 2n$	
4 <i>d</i> $\bar{6}$. .	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$			$hkil$: $l = 2n$	
4 <i>c</i> 3.2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$			$hkil$: $l = 2n$	
2 <i>b</i> 6/ <i>m</i> . .	$0, 0, 0$	$0, 0, \frac{1}{2}$					$hkil$: $l = 2n$	
2 <i>a</i> 622	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					$hkil$: $l = 2n$	

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [100] $p2mm$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x, 0, 0

Along [210] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, \frac{1}{2}x, 0$

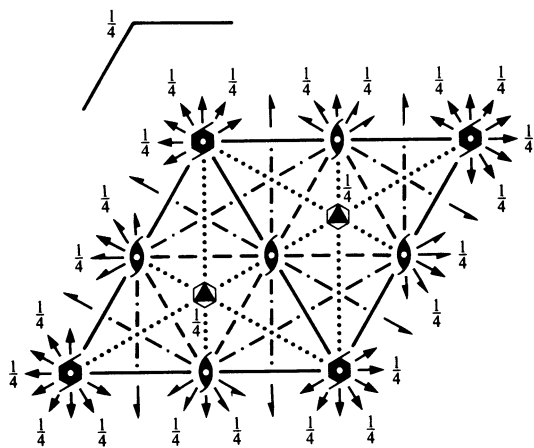
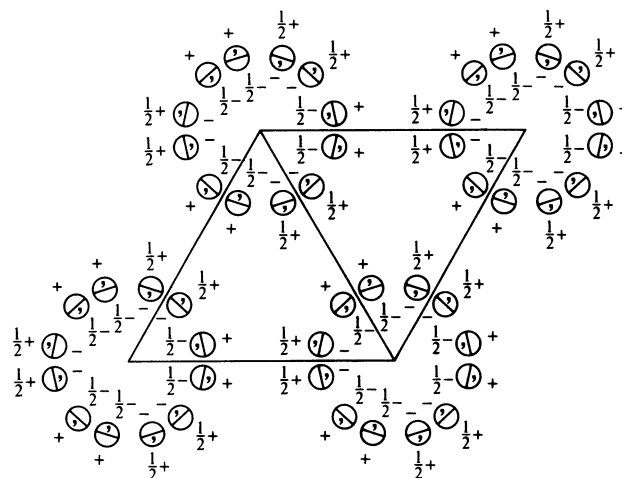
(Continued on preceding page)

$P6_3/mcm$
 D_{6h}^3
 $6/mmm$

Hexagonal

No. 193

 $P 6_3/m 2/c 2/m$

 Patterson symmetry $P6/mmm$

 For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)

Origin at centre ($\bar{3}1m$) at $\bar{3}c2/m$
Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$; $x \leq (1+y)/2$; $y \leq \min(1-x, x)$
Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 $0, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$
Symmetry operations

- | | | |
|------------------------------------|---|---|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2}) 0, 0, z$ | (5) $6^-(0, 0, \frac{1}{2}) 0, 0, z$ | (6) $6^+(0, 0, \frac{1}{2}) 0, 0, z$ |
| (7) $2 x, x, \frac{1}{4}$ | (8) $2 x, 0, \frac{1}{4}$ | (9) $2 0, y, \frac{1}{4}$ |
| (10) $2 x, \bar{x}, 0$ | (11) $2 x, 2x, 0$ | (12) $2 2x, x, 0$ |
| (13) $\bar{1} 0, 0, 0$ | (14) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (15) $\bar{3}^- 0, 0, z; 0, 0, 0$ |
| (16) $m x, y, \frac{1}{4}$ | (17) $\bar{6}^- 0, 0, z; 0, 0, \frac{1}{4}$ | (18) $\bar{6}^+ 0, 0, z; 0, 0, \frac{1}{4}$ |
| (19) $c x, \bar{x}, z$ | (20) $c x, 2x, z$ | (21) $c 2x, x, z$ |
| (22) $m x, x, z$ | (23) $m x, 0, z$ | (24) $m 0, y, z$ |

Maximal non-isomorphic subgroups

- | | |
|----------------------------------|---|
| I [2] $P\bar{6}2m$ (189) | 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24 |
| [2] $P\bar{6}c2$ (188) | 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21 |
| [2] $P6_3cm$ (185) | 1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24 |
| [2] $P6_322$ (182) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12 |
| [2] $P6_3/m11$ ($P6_3/m$, 176) | 1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18 |
| [2] $P\bar{3}c1$ (165) | 1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21 |
| [2] $P\bar{3}1m$ (162) | 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24 |
| { [3] $Pmcm$ ($Cmcm$, 63) | 1; 4; 7; 10; 13; 16; 19; 22 |
| [3] $Pmcm$ ($Cmcm$, 63) | 1; 4; 8; 11; 13; 16; 20; 23 |
| [3] $Pmcm$ ($Cmcm$, 63) | 1; 4; 9; 12; 13; 16; 21; 24 |

IIa none

IIb [3] $H6_3/mcm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3/mmc$, 194)

Maximal isomorphic subgroups of lowest index
IIc [3] $P6_3/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (193); [4] $P6_3/mcm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (193)

Minimal non-isomorphic supergroups
I none

II [3] $H6_3/mcm$ ($P6_3/mmc$, 194); [2] $P6/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (191)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
24 <i>l</i> 1	(1) x, y, z (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (10) $\bar{y}, \bar{x}, \bar{z}$ (13) $\bar{x}, \bar{y}, \bar{z}$ (16) $x, y, \bar{z} + \frac{1}{2}$ (19) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (22) y, x, z	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (8) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$ (11) $\bar{x} + y, y, \bar{z}$ (14) $y, \bar{x} + y, \bar{z}$ (17) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$ (20) $\bar{x} + y, y, z + \frac{1}{2}$ (23) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z + \frac{1}{2}$ (9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$ (12) $x, x - y, \bar{z}$ (15) $x - y, x, \bar{z}$ (18) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$ (21) $x, x - y, z + \frac{1}{2}$ (24) $\bar{x}, \bar{x} + y, z$				General: $h\bar{h}0l : l = 2n$ $000l : l = 2n$
12 <i>k</i> $\dots m$	$x, 0, z$ $0, \bar{x}, z + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$	$0, x, z$ $x, x, z + \frac{1}{2}$ $0, \bar{x}, \bar{z}$	\bar{x}, \bar{x}, z $0, x, \bar{z} + \frac{1}{2}$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z + \frac{1}{2}$ $x, 0, \bar{z} + \frac{1}{2}$ x, x, \bar{z}			Special: as above, plus no extra conditions
12 <i>j</i> $m \dots$	$x, y, \frac{1}{4}$ $y, x, \frac{1}{4}$	$\bar{y}, x - y, \frac{1}{4}$ $x - y, \bar{y}, \frac{1}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{x} + y, \frac{1}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{y}, \bar{x}, \frac{3}{4}$	$y, \bar{x} + y, \frac{3}{4}$ $\bar{x} + y, y, \frac{3}{4}$	$x - y, x, \frac{3}{4}$ $x, x - y, \frac{3}{4}$	no extra conditions
12 <i>i</i> $\dots 2$	$x, 2x, 0$ $\bar{x}, 2\bar{x}, 0$	$2\bar{x}, \bar{x}, 0$ $2x, x, 0$	$x, \bar{x}, 0$ $\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, \frac{1}{2}$ $x, 2x, \frac{1}{2}$	$2x, x, \frac{1}{2}$ $2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$ $x, \bar{x}, \frac{1}{2}$	$hkil : l = 2n$
8 <i>h</i> $3 \dots$	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \bar{z} + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$ $\frac{2}{3}, \frac{1}{3}, z$			$hkil : l = 2n$
6 <i>g</i> $m 2 m$	$x, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	no extra conditions
6 <i>f</i> $\dots 2/m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil : l = 2n$
4 <i>e</i> $3 \dots m$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$			$hkil : l = 2n$
4 <i>d</i> $3 \dots 2$	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, 0$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$			$hkil : l = 2n$
4 <i>c</i> $\bar{6} \dots$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$			$hkil : l = 2n$
2 <i>b</i> $\bar{3} \dots m$	$0, 0, 0$	$0, 0, \frac{1}{2}$					$hkil : l = 2n$
2 <i>a</i> $\bar{6} 2 m$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					$hkil : l = 2n$

Symmetry of special projectionsAlong $[001] p6mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along $[100] p2mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, 0, 0$ Along $[210] p2gm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

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$P6_3/mmc$

D_{6h}^4

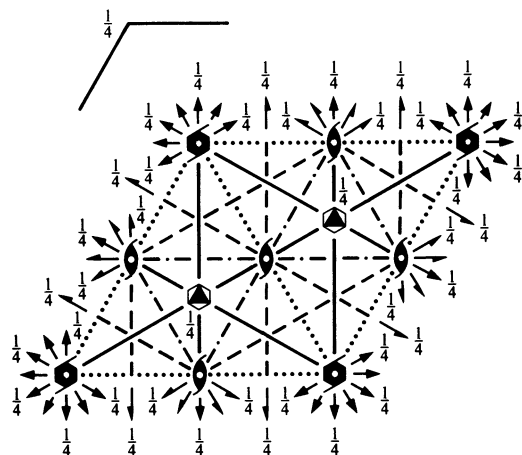
$6/mmm$

Hexagonal

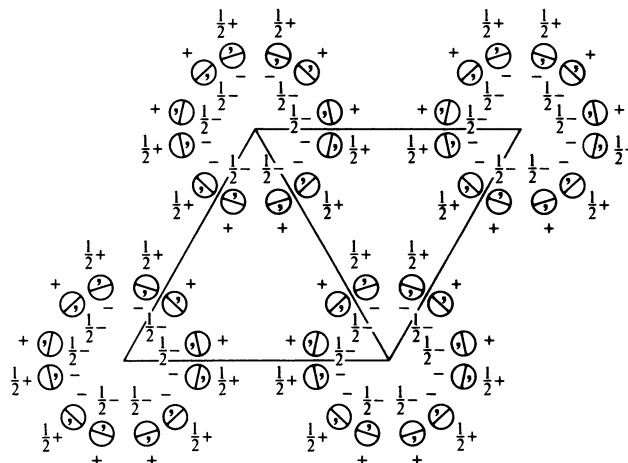
No. 194

$P 6_3/m 2/m 2/c$

Patterson symmetry $P6/mmm$



For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)



Origin at centre ($\bar{3}m1$) at $\bar{3}2/mc$

Asymmetric unit $0 \leq x \leq \frac{2}{3}; 0 \leq y \leq \frac{2}{3}; 0 \leq z \leq \frac{1}{4}; x \leq 2y; y \leq \min(1-x, 2x)$

Vertices $0, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
 $0, 0, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$

Symmetry operations

- | | | |
|------------------------------------|---|---|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2(0, 0, \frac{1}{2}) 0, 0, z$ | (5) $6^-(0, 0, \frac{1}{2}) 0, 0, z$ | (6) $6^+(0, 0, \frac{1}{2}) 0, 0, z$ |
| (7) $2 x, x, 0$ | (8) $2 x, 0, 0$ | (9) $2 0, y, 0$ |
| (10) $2 x, \bar{x}, \frac{1}{4}$ | (11) $2 x, 2x, \frac{1}{4}$ | (12) $2 2x, x, \frac{1}{4}$ |
| (13) $\bar{1} 0, 0, 0$ | (14) $\bar{3}^+ 0, 0, z; 0, 0, 0$ | (15) $\bar{3}^- 0, 0, z; 0, 0, 0$ |
| (16) $m x, y, \frac{1}{4}$ | (17) $\bar{6}^- 0, 0, z; 0, 0, \frac{1}{4}$ | (18) $\bar{6}^+ 0, 0, z; 0, 0, \frac{1}{4}$ |
| (19) $m x, \bar{x}, z$ | (20) $m x, 2x, z$ | (21) $m 2x, x, z$ |
| (22) $c x, x, z$ | (23) $c x, 0, z$ | (24) $c 0, y, z$ |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{6}2c$ (190) 1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
 [2] $P\bar{6}m2$ (187) 1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
 [2] $P6_3mc$ (186) 1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
 [2] $P6_322$ (182) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
 [2] $P6_3/m11$ ($P6_3/m$, 176) 1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
 [2] $P\bar{3}m1$ (164) 1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
 [2] $P\bar{3}1c$ (163) 1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
 { [3] $Pm\bar{6}c$ ($Cm\bar{6}c$, 63) 1; 4; 7; 10; 13; 16; 19; 22
 [3] $Pm\bar{6}c$ ($Cm\bar{6}c$, 63) 1; 4; 8; 11; 13; 16; 20; 23
 [3] $Pm\bar{6}c$ ($Cm\bar{6}c$, 63) 1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb [3] $H6_3/mmc$ ($a' = 3a, b' = 3b$) ($P6_3/mcm$, 193)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/mmc$ ($c' = 3c$) (194); [4] $P6_3/mmc$ ($a' = 2a, b' = 2b$) (194)

Minimal non-isomorphic supergroups

I none

II [3] $H6_3/mmc$ ($P6_3/mcm$, 193); [2] $P6/mmm$ ($c' = \frac{1}{2}c$) (191)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
24 <i>l</i> 1	(1) x, y, z (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (7) y, x, \bar{z} (10) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (13) $\bar{x}, \bar{y}, \bar{z}$ (16) $x, y, \bar{z} + \frac{1}{2}$ (19) \bar{y}, \bar{x}, z (22) $y, x, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (8) $x - y, \bar{y}, \bar{z}$ (11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$ (14) $y, \bar{x} + y, \bar{z}$ (17) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$ (20) $\bar{x} + y, y, z$ (23) $x - y, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z + \frac{1}{2}$ (9) $\bar{x}, \bar{x} + y, \bar{z}$ (12) $x, x - y, \bar{z} + \frac{1}{2}$ (15) $x - y, x, \bar{z}$ (18) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$ (21) $x, x - y, z$ (24) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$				General: $hh\bar{2}hl$: $l = 2n$ $000l$: $l = 2n$
12 <i>k</i> . <i>m</i> .	$x, 2x, z$ $2x, x, z + \frac{1}{2}$ \bar{x}, x, \bar{z}	$2\bar{x}, \bar{x}, z$ $\bar{x}, x, z + \frac{1}{2}$ $2\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$	x, \bar{x}, z $2x, x, \bar{z}$ $x, 2x, \bar{z} + \frac{1}{2}$	$\bar{x}, 2\bar{x}, z + \frac{1}{2}$ $\bar{x}, 2\bar{x}, \bar{z}$ $x, \bar{x}, \bar{z} + \frac{1}{2}$			Special: as above, plus no extra conditions
12 <i>j</i> <i>m</i> . .	$x, y, \frac{1}{4}$ $y, x, \frac{3}{4}$	$\bar{y}, x - y, \frac{1}{4}$ $x - y, \bar{y}, \frac{3}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{x} + y, \frac{3}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{y}, \bar{x}, \frac{1}{4}$	$y, \bar{x} + y, \frac{3}{4}$ $\bar{x} + y, y, \frac{1}{4}$	$x - y, x, \frac{3}{4}$ $x, x - y, \frac{1}{4}$	no extra conditions
12 <i>i</i> . 2 .	$x, 0, 0$ $\bar{x}, 0, 0$	$0, x, 0$ $0, \bar{x}, 0$	$\bar{x}, \bar{x}, 0$ $x, x, 0$	$\bar{x}, 0, \frac{1}{2}$ $x, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $0, x, \frac{1}{2}$	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$	$hkil$: $l = 2n$
6 <i>h</i> <i>m m</i> 2	$x, 2x, \frac{1}{4}$	$2\bar{x}, \bar{x}, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$	$\bar{x}, 2\bar{x}, \frac{3}{4}$	$2x, x, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$	no extra conditions
6 <i>g</i> . 2/ <i>m</i> .	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil$: $l = 2n$
4 <i>f</i> 3 <i>m</i> .	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$			$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> 3 <i>m</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$			$hkil$: $l = 2n$
2 <i>d</i> $\bar{6}m$ 2	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	}				$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> $\bar{6}m$ 2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$					
2 <i>b</i> $\bar{6}m$ 2	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					$hkil$: $l = 2n$
2 <i>a</i> $\bar{3}m$.	$0, 0, 0$	$0, 0, \frac{1}{2}$					$hkil$: $l = 2n$

Symmetry of special projectionsAlong [001] $p6mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z Along [100] $p2gm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, 0, 0$ Along [210] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

(Continued on preceding page)

*P*23

T^1

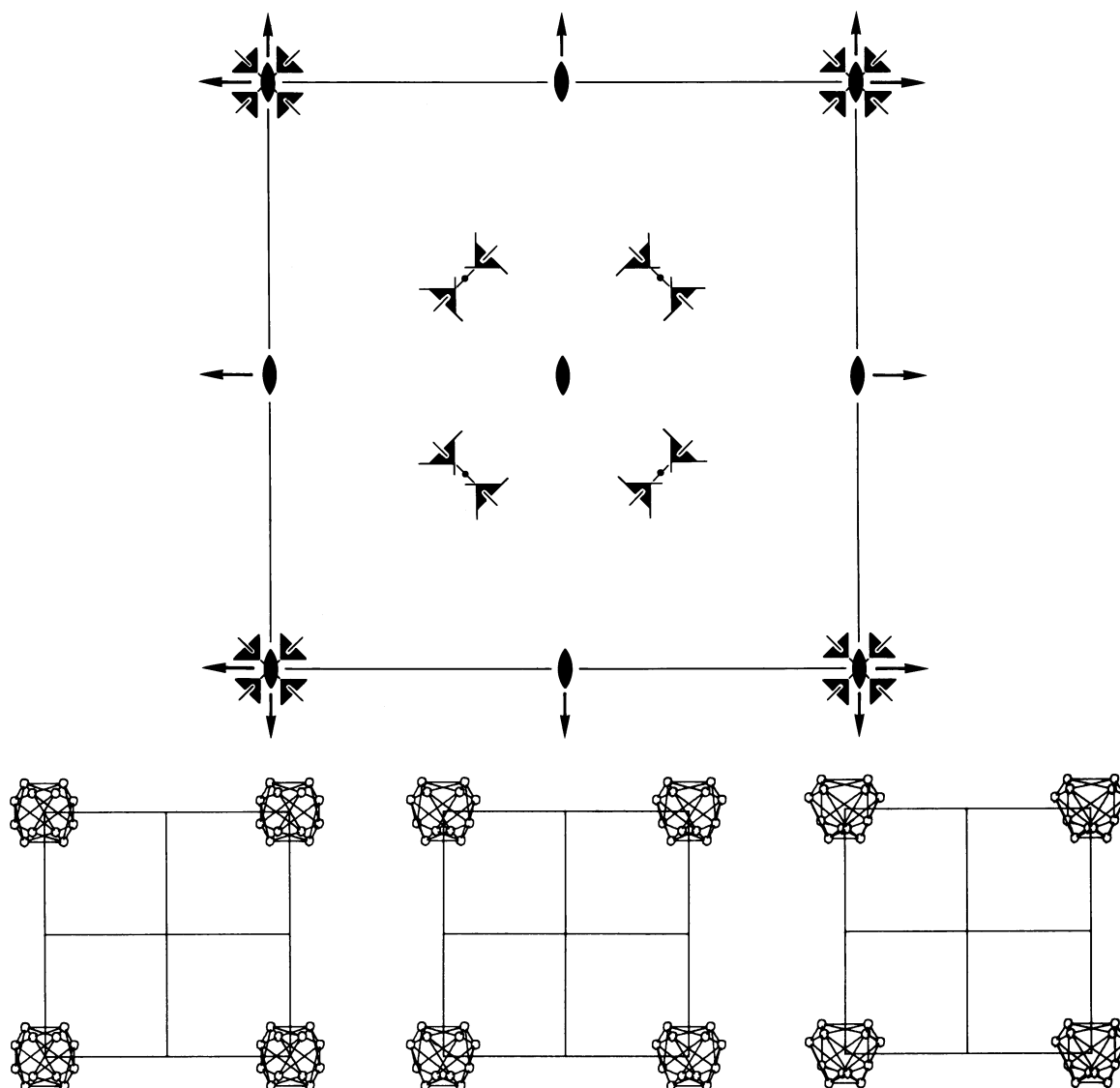
23

Cubic

No. 195

*P*23

Patterson symmetry $Pm\bar{3}$



Origin at 23

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}; y \leq 1-x; z \leq \min(x,y)$

Vertices $0,0,0 \ 1,0,0 \ 0,1,0 \ \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------|--------------------------------|--------------------------------|--------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) 3^+ x,x,x | (6) 3^+ \bar{x},x,\bar{x} | (7) 3^+ x,\bar{x},\bar{x} | (8) 3^+ \bar{x},\bar{x},x |
| (9) 3^- x,x,x | (10) 3^- x,\bar{x},\bar{x} | (11) 3^- \bar{x},\bar{x},x | (12) 3^- \bar{x},x,\bar{x} |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions	
						h, k, l cyclically permutable	
						General:	
12	j 1	(1) x, y, z (5) z, x, y (9) y, z, x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x	no conditions	
						Special: no extra conditions	
6	i 2..	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
6	h 2..	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$
6	g 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$0, \frac{1}{2}, x$	$0, \frac{1}{2}, \bar{x}$
6	f 2..	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
4	e .3.	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
3	d 222..	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$			
3	c 222..	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
1	b 23.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
1	a 23.	$0, 0, 0$					

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0, 0, z	Along [111] $p3$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along [110] $p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$
--	---	---

Maximal non-isomorphic subgroups

I	[3] $P21$ ($P222, 16$)	1; 2; 3; 4
{	[4] $P13$ ($R3, 146$)	1; 5; 9
	[4] $P13$ ($R3, 146$)	1; 6; 12
	[4] $P13$ ($R3, 146$)	1; 7; 10
	[4] $P13$ ($R3, 146$)	1; 8; 11

IIa none

IIb [2] $F23$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (196); [4] $I2_13$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (199); [4] $I23$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (197)

Maximal isomorphic subgroups of lowest index

IIc [27] $P23$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (195)

Minimal non-isomorphic supergroups

I	[2] $Pm\bar{3}$ (200); [2] $Pn\bar{3}$ (201); [2] $P432$ (207); [2] $P4_232$ (208); [2] $P\bar{4}3m$ (215); [2] $P\bar{4}3n$ (218)
II	[2] $I23$ (197); [4] $F23$ (196)

F 23

T^2

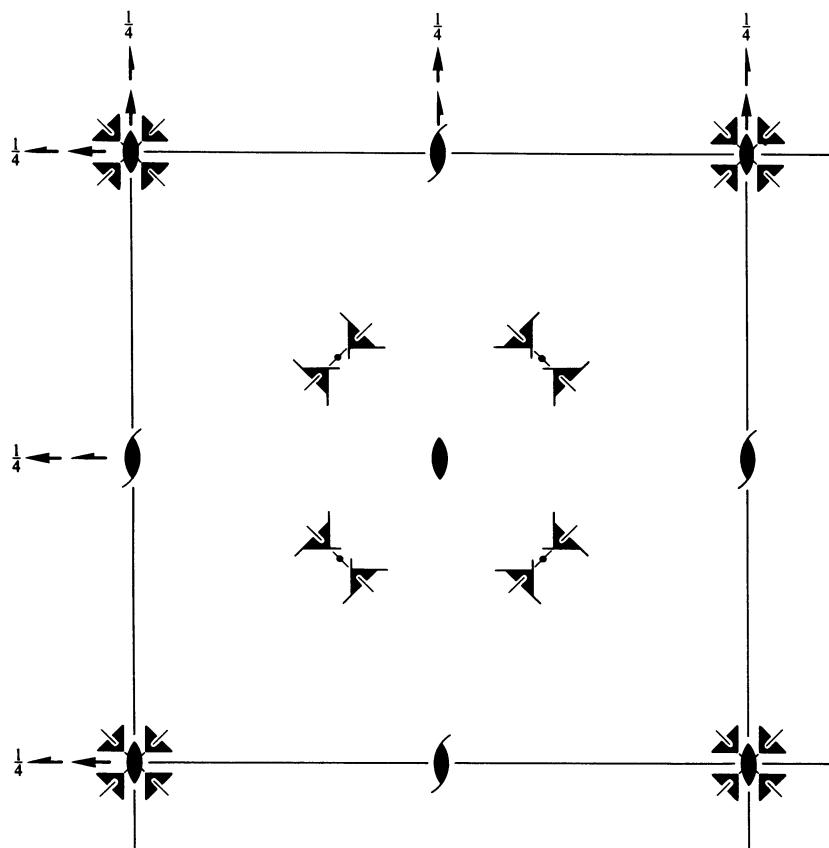
23

Cubic

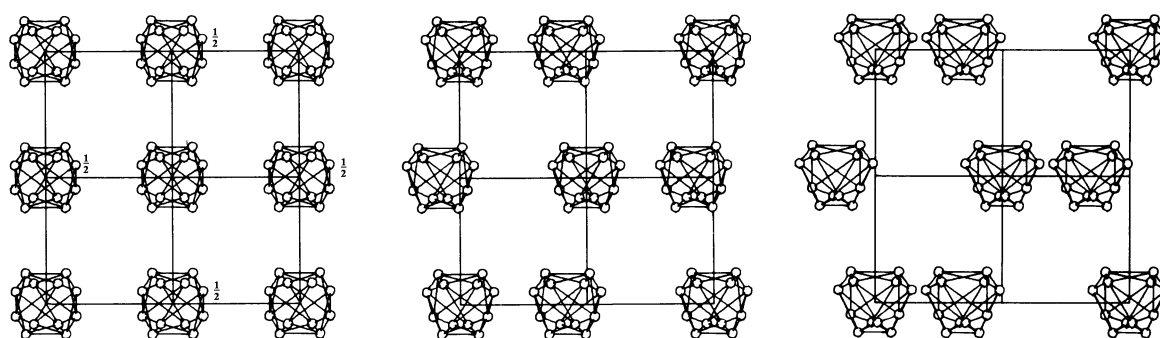
No. 196

F 23

Patterson symmetry $Fm\bar{3}$



Upper left quadrant only



Origin at 23

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq x; \max(x - \frac{1}{2}, -y) \leq z \leq \min(\frac{1}{2} - x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--------------------------|--|--|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x} ,x, \bar{x} | (7) 3 ⁺ x, \bar{x} , \bar{x} | (8) 3 ⁺ \bar{x} , \bar{x} ,x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x} , \bar{x} | (11) 3 ⁻ \bar{x} , \bar{x} ,x | (12) 3 ⁻ \bar{x} ,x, \bar{x} |

For (0, $\frac{1}{2}$, $\frac{1}{2}$)+ set

- | | | | |
|--|---|--|---|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) 0, $\frac{1}{4}$,z | (3) 2(0, $\frac{1}{2}$,0) 0,y, $\frac{1}{4}$ | (4) 2 x, $\frac{1}{4}$, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x- $\frac{1}{3}$,x- $\frac{1}{6}$,x | (6) 3 ⁺ \bar{x} ,x+ $\frac{1}{2}$, \bar{x} | (7) 3 ⁺ (- $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x+ $\frac{1}{3}$, \bar{x} - $\frac{1}{6}$, \bar{x} | (8) 3 ⁺ \bar{x} , \bar{x} + $\frac{1}{2}$,x |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x- $\frac{1}{6}$,x+ $\frac{1}{6}$,x | (10) 3 ⁻ (- $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x+ $\frac{1}{6}$, \bar{x} + $\frac{1}{6}$, \bar{x} | (11) 3 ⁻ \bar{x} + $\frac{1}{2}$, \bar{x} + $\frac{1}{2}$,x | (12) 3 ⁻ \bar{x} - $\frac{1}{2}$,x+ $\frac{1}{2}$, \bar{x} |

For ($\frac{1}{2}$,0, $\frac{1}{2}$)+ set

- | | | | |
|--|---|---|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}$,0,z | (3) 2 $\frac{1}{4}$,y, $\frac{1}{4}$ | (4) 2($\frac{1}{2}$,0,0) x,0, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x+ $\frac{1}{6}$,x- $\frac{1}{6}$,x | (6) 3 ⁺ ($\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$) \bar{x} + $\frac{1}{6}$,x+ $\frac{1}{6}$, \bar{x} | (7) 3 ⁺ x+ $\frac{1}{2}$, \bar{x} - $\frac{1}{2}$, \bar{x} | (8) 3 ⁺ \bar{x} + $\frac{1}{2}$, \bar{x} + $\frac{1}{2}$,x |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x- $\frac{1}{6}$,x- $\frac{1}{3}$,x | (10) 3 ⁻ x+ $\frac{1}{2}$, \bar{x} , \bar{x} | (11) 3 ⁻ \bar{x} + $\frac{1}{2}$, \bar{x} ,x | (12) 3 ⁻ ($\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$) \bar{x} - $\frac{1}{6}$,x+ $\frac{1}{3}$, \bar{x} |

For ($\frac{1}{2}$, $\frac{1}{2}$,0)+ set

- | | | | |
|--|--|---|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}$, $\frac{1}{4}$,z | (3) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}$,y,0 | (4) 2($\frac{1}{2}$,0,0) x, $\frac{1}{4}$,0 |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x+ $\frac{1}{6}$,x+ $\frac{1}{3}$,x | (6) 3 ⁺ \bar{x} + $\frac{1}{2}$,x, \bar{x} | (7) 3 ⁺ x+ $\frac{1}{2}$, \bar{x} , \bar{x} | (8) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}$) \bar{x} + $\frac{1}{6}$, \bar{x} + $\frac{1}{3}$,x |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x+ $\frac{1}{3}$,x+ $\frac{1}{6}$,x | (10) 3 ⁻ x, \bar{x} + $\frac{1}{2}$, \bar{x} | (11) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}$) \bar{x} + $\frac{1}{3}$, \bar{x} + $\frac{1}{6}$,x | (12) 3 ⁻ \bar{x} ,x+ $\frac{1}{2}$, \bar{x} |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+	($\frac{1}{2}$,0, $\frac{1}{2}$)+	($\frac{1}{2}$, $\frac{1}{2}$,0)+		
48 h 1	(1) x,y,z (5) z,x,y (9) y,z,x	(2) \bar{x} , \bar{y} ,z (6) z, \bar{x} , \bar{y} (10) \bar{y} ,z, \bar{x}	(3) \bar{x} ,y, \bar{z} (7) \bar{z} , \bar{x} ,y (11) y, \bar{z} , \bar{x}	(4) x, \bar{y} , \bar{z} (8) \bar{z} ,x, \bar{y} (12) \bar{y} , \bar{z} ,x	<i>hkl</i> : $h+k, h+l, k+l = 2n$ <i>Ok</i> l : $k, l = 2n$ <i>hh</i> l : $h+l = 2n$ <i>h00</i> : $h = 2n$	
24 g 2..	x, $\frac{1}{4}$, $\frac{1}{4}$	\bar{x} , $\frac{3}{4}$, $\frac{1}{4}$	$\frac{1}{4}$, x, $\frac{1}{4}$	$\frac{1}{4}$, \bar{x} , $\frac{3}{4}$	$\frac{1}{4}$, $\frac{1}{4}$, x	$\frac{3}{4}$, $\frac{1}{4}$, \bar{x}
24 f 2..	x,0,0	\bar{x} ,0,0	0,x,0	0, \bar{x} ,0	0,0,x	0,0, \bar{x}
16 e .3.	x,x,x	\bar{x} , \bar{x} ,x	\bar{x} ,x, \bar{x}	x, \bar{x} , \bar{x}		
4 d 23.	$\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$					
4 c 23.	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$					
4 b 23.	$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$					
4 a 23.	0,0,0					

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ Origin at 0,0,z	Along [111] $p3$ $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x,x,x	Along [110] $c1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at x,x,0
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Maximal non-isomorphic subgroups

- I** [3] $F 21 (F 222, 22)$ (1; 2; 3; 4)+
 { [4] $F 13 (R3, 146)$ (1; 5; 9)+
 [4] $F 13 (R3, 146)$ (1; 6; 12)+
 [4] $F 13 (R3, 146)$ (1; 7; 10)+
 [4] $F 13 (R3, 146)$ (1; 8; 11)+
- IIa** { [4] $P 2_1 3 (198)$ 1; 5; 9; (2; 7; 12) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 7; 10; (2; 5; 11) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 8; 11; (2; 6; 10) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 6; 12; (2; 8; 9) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 5; 9; (3; 8; 10) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 7; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 7; 10; (3; 6; 9) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 5; 11) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 8; 11; (3; 5; 12) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 6; 10) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 2_1 3 (198)$ 1; 6; 12; (3; 7; 11) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 8; 9) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
 [4] $P 23 (195)$ 1; 2; 3; 4; (5; 6; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (9; 10; 11; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (9; 10; 11; 12) + $(0, \frac{1}{2}, \frac{1}{2})$
 [4] $P 23 (195)$ 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (9; 10; 11; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$
 [4] $P 23 (195)$ 1; 5; 9; (4; 6; 11) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 7; 12) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 7; 10; (4; 8; 12) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 5; 11) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 8; 11; (4; 7; 9) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 6; 10) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 [4] $P 23 (195)$ 1; 6; 12; (4; 5; 10) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 8; 9) + $(\frac{1}{2}, \frac{1}{2}, 0)$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F 23 (a' = 3a, b' = 3b, c' = 3c)$ (196)

Minimal non-isomorphic supergroups

I [2] $F m \bar{3} (202)$; [2] $F d \bar{3} (203)$; [2] $F 4 3 2 (209)$; [2] $F 4_1 3 2 (210)$; [2] $F \bar{4} 3 m (216)$; [2] $F \bar{4} 3 c (219)$

II [2] $P 23 (a' = \frac{1}{2}c, b' = \frac{1}{2}b, c' = \frac{1}{2}c)$ (195)

*I*23

T^3

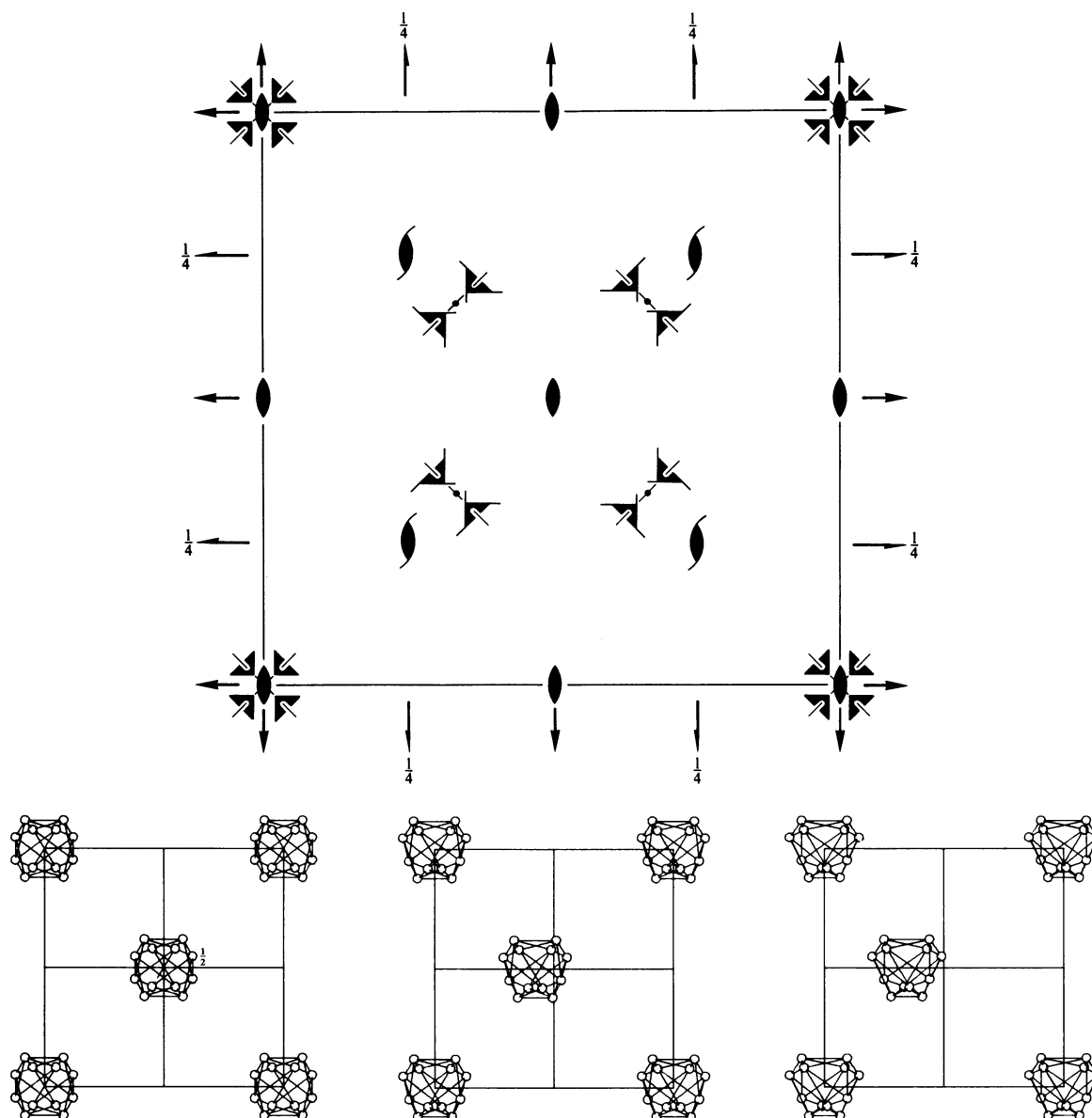
23

Cubic

No. 197

*I*23

Patterson symmetry $Im\bar{3}$



Origin at 23

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \min(x, 1-x); z \leq y$
Vertices $0,0,0 \quad 1,0,0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--------------------------|--|--|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x} ,x, \bar{x} | (7) 3 ⁺ x, \bar{x} , \bar{x} | (8) 3 ⁺ \bar{x} , \bar{x} ,x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x} , \bar{x} | (11) 3 ⁻ \bar{x} , \bar{x} ,x | (12) 3 ⁻ \bar{x} ,x, \bar{x} |

For ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2($\frac{1}{2}$,0,0) $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x | (6) 3 ⁺ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$ | (7) 3 ⁺ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$ | (8) 3 ⁺ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$ |
| (9) 3 ⁻ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x | (10) 3 ⁻ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$ | (11) 3 ⁻ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$ | (12) 3 ⁻ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions	
		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				h, k, l cyclically permutable General:	
24	f 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}	$hkl : h + k + l = 2n$	
		(5) z, x, y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}	$0kl : k + l = 2n$	
		(9) y, z, x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x	$hhl : l = 2n$	
						$h00 : h = 2n$	
						Special: no extra conditions	
12	e 2..	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$
12	d 2..	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
8	c .3.	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
6	b 222..	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	a 23.	$0, 0, 0$					

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [111] $p3$

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$

Origin at x, x, x

$\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$

Along [110] $p1m1$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$

Origin at $x, x, 0$

$\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Maximal non-isomorphic subgroups

I [3] $I21 (I222, 23)$ (1; 2; 3; 4)+

{ [4] $I13 (R3, 146)$ (1; 5; 9)+
[4] $I13 (R3, 146)$ (1; 6; 12)+
[4] $I13 (R3, 146)$ (1; 7; 10)+
[4] $I13 (R3, 146)$ (1; 8; 11)+

IIa [2] $P23 (195)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $I23 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (197)$

Minimal non-isomorphic supergroups

I [2] $Im\bar{3} (204)$; [2] $I432 (211)$; [2] $I\bar{4}3m (217)$

II [4] $P23 (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (195)$

$P2_13$

T^4

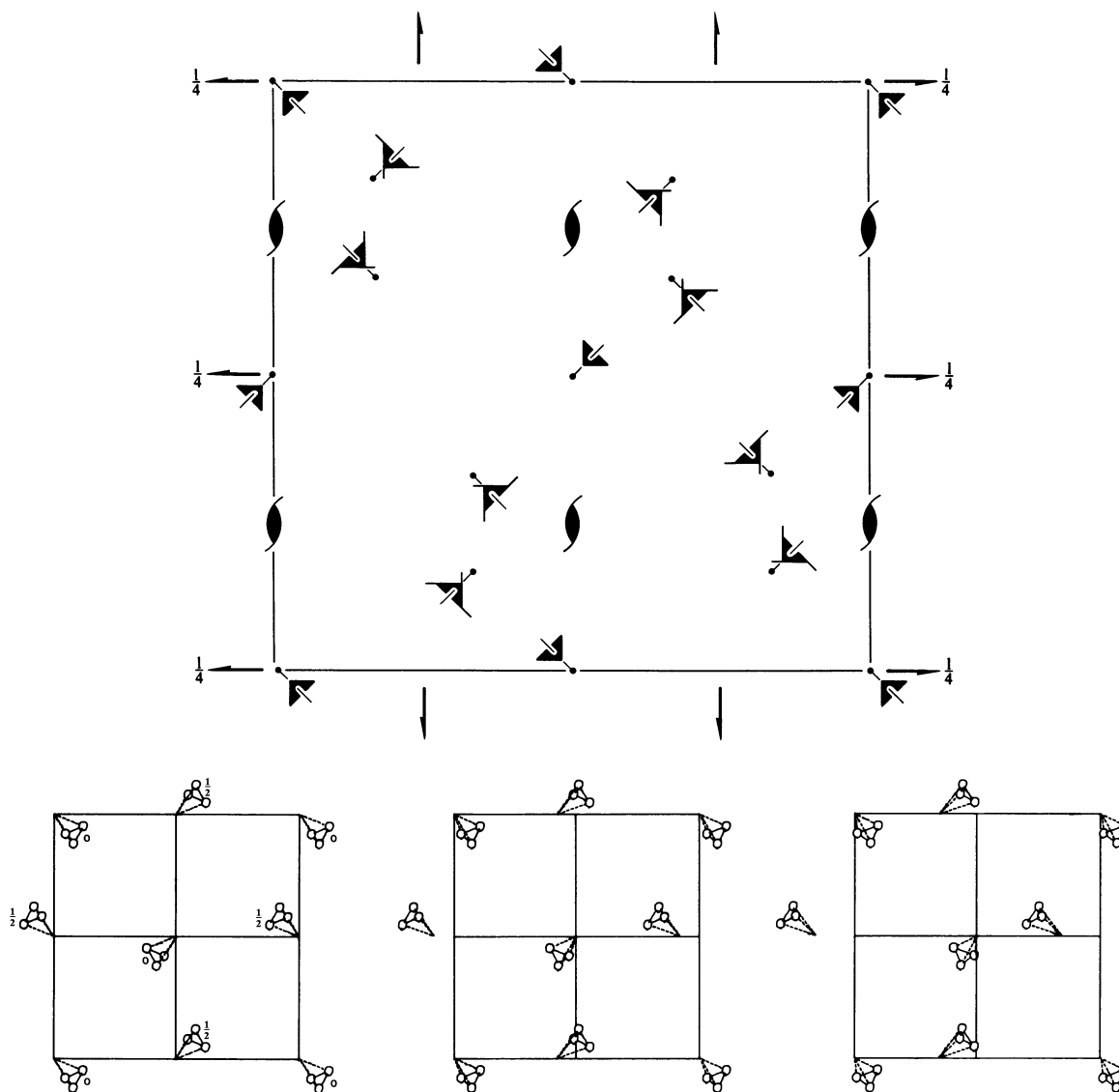
23

Cubic

No. 198

$P2_13$

Patterson symmetry $Pm\bar{3}$



Origin on $3[111]$ at midpoint of three non-intersecting pairs of parallel 2₁ axes

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; -\frac{1}{2} \leq z \leq \frac{1}{2}; \max(x - \frac{1}{2}, -y) \leq z \leq \min(x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \quad 0, \frac{1}{2}, -\frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------|---|---|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- (\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					h, k, l cyclically permutable
					General:
12 <i>b</i> 1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	$h00: h = 2n$
	(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$	(7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$	(8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$	
	(9) y, z, x	(10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$	(12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$	
					Special: no extra conditions
4 <i>a</i> .3.	x, x, x	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$	

Symmetry of special projections

Along [001] $p2gg$	Along [111] $p3$	Along [110] $p1g1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $\frac{1}{4}, 0, z$	Origin at x, x, x	Origin at $x + \frac{1}{4}, x, 0$

Maximal non-isomorphic subgroups

I	[3] $P2_11 (P2_12_12_1, 19)$	1; 2; 3; 4
{	[4] $P13 (R3, 146)$	1; 5; 9
	[4] $P13 (R3, 146)$	1; 6; 12
	[4] $P13 (R3, 146)$	1; 7; 10
	[4] $P13 (R3, 146)$	1; 8; 11

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $P2_13 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (198)$

Minimal non-isomorphic supergroups

I [2] $Pa\bar{3} (205)$; [2] $P4_332 (212)$; [2] $P4_332 (213)$

II [2] $I2_13 (199)$; [4] $F23 (196)$

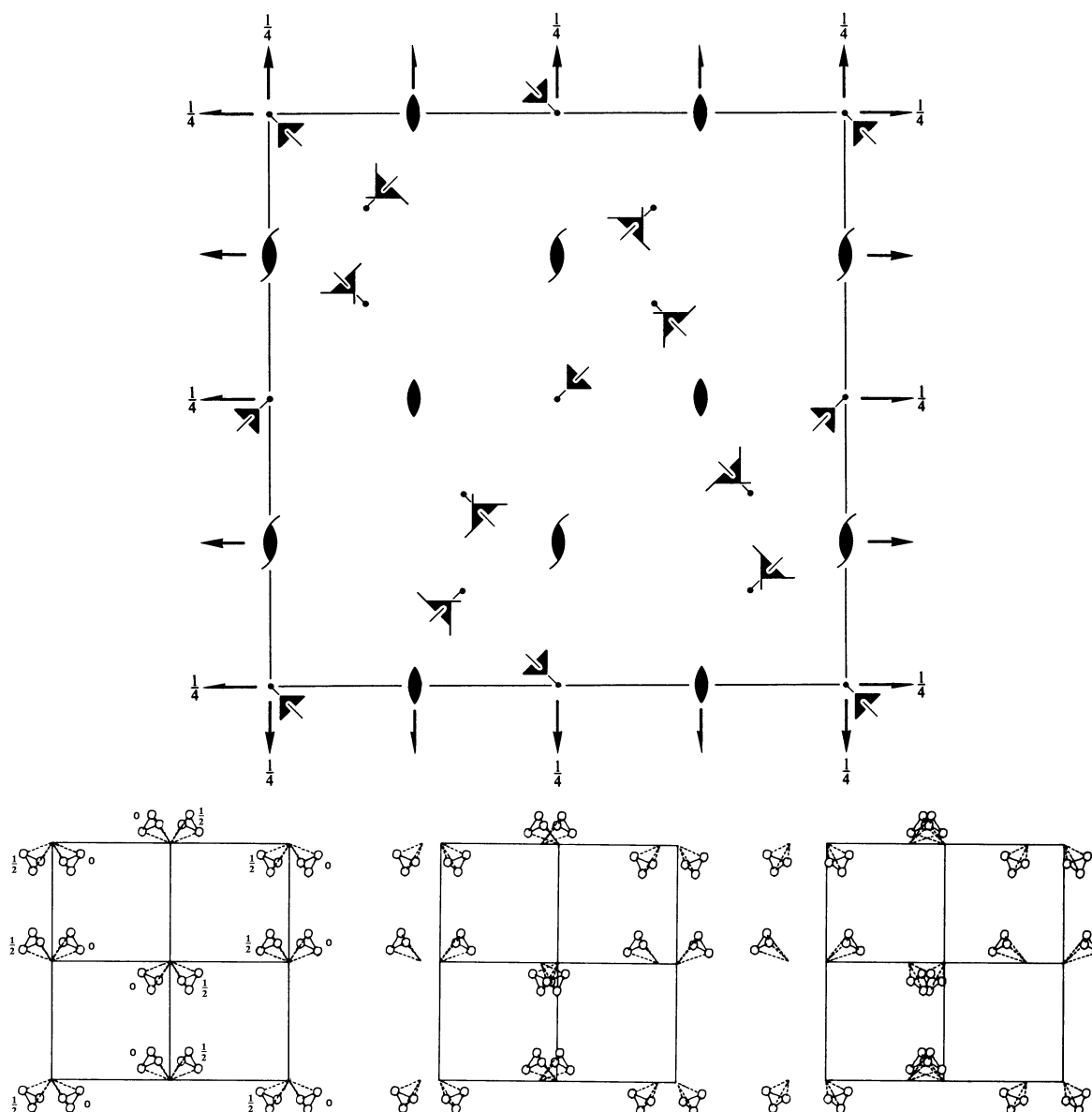
$I2_13$
 T^5

23

Cubic

No. 199

 $I2_13$

 Patterson symmetry $Im\bar{3}$


Origin on $3[111]$ at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2₁ axes

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $z \leq \min(x, y)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

For $(0, 0, 0)$ + set

- | | | | |
|---------------------|---|--|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) 3^+ x, x, x | (6) 3^+ $\bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) 3^+ $x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) 3^+ $\bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) 3^- x, x, x | (10) 3^- $(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) 3^- $(\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) 3^- $(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2 $0, \frac{1}{4}, z$ | (3) 2 $\frac{1}{4}, y, 0$ | (4) 2 $x, 0, \frac{1}{4}$ |
| (5) 3^+ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, x | (6) 3^+ $(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ | (7) 3^+ $(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (8) 3^+ $(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ |
| (9) 3^- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, x | (10) 3^- $(\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) 3^- $(-\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) 3^- $(-\frac{1}{6}, \frac{1}{6}, -\frac{1}{6})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions		
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$				h, k, l cyclically permutable General:		
24 <i>c</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$ (10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$ $OkI : k + l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$		
12 <i>b</i> 2..	$x, 0, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, 0, \frac{3}{4}$	$\frac{1}{4}, x, 0$	$\frac{3}{4}, \bar{x} + \frac{1}{2}, 0$	$0, \frac{1}{4}, x$	$0, \frac{3}{4}, \bar{x} + \frac{1}{2}$	Special: no extra conditions
8 <i>a</i> .3.	x, x, x	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$			

Symmetry of special projections

Along $[001] c2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $\frac{1}{4}, 0, z$	Along $[111] p3$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along $[110] p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, x + \frac{1}{4}, 0$
--	---	--

Maximal non-isomorphic subgroups

I	$[3] I2_1 1 (I2_1 2_1 2_1, 24)$	$(1; 2; 3; 4) +$
{	$[4] I13 (R3, 146)$	$(1; 5; 9) +$
	$[4] I13 (R3, 146)$	$(1; 6; 12) +$
	$[4] I13 (R3, 146)$	$(1; 7; 10) +$
	$[4] I13 (R3, 146)$	$(1; 8; 11) +$
IIa	$[2] P2_1 3 (198)$	$1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc $[27] I2_1 3 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (199)$

Minimal non-isomorphic supergroups

I	$[2] Ia\bar{3} (206); [2] I4_1 32 (214); [2] I\bar{4} 3d (220)$
II	$[4] P23 (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (195)$

$Pm\bar{3}$

T_h^1

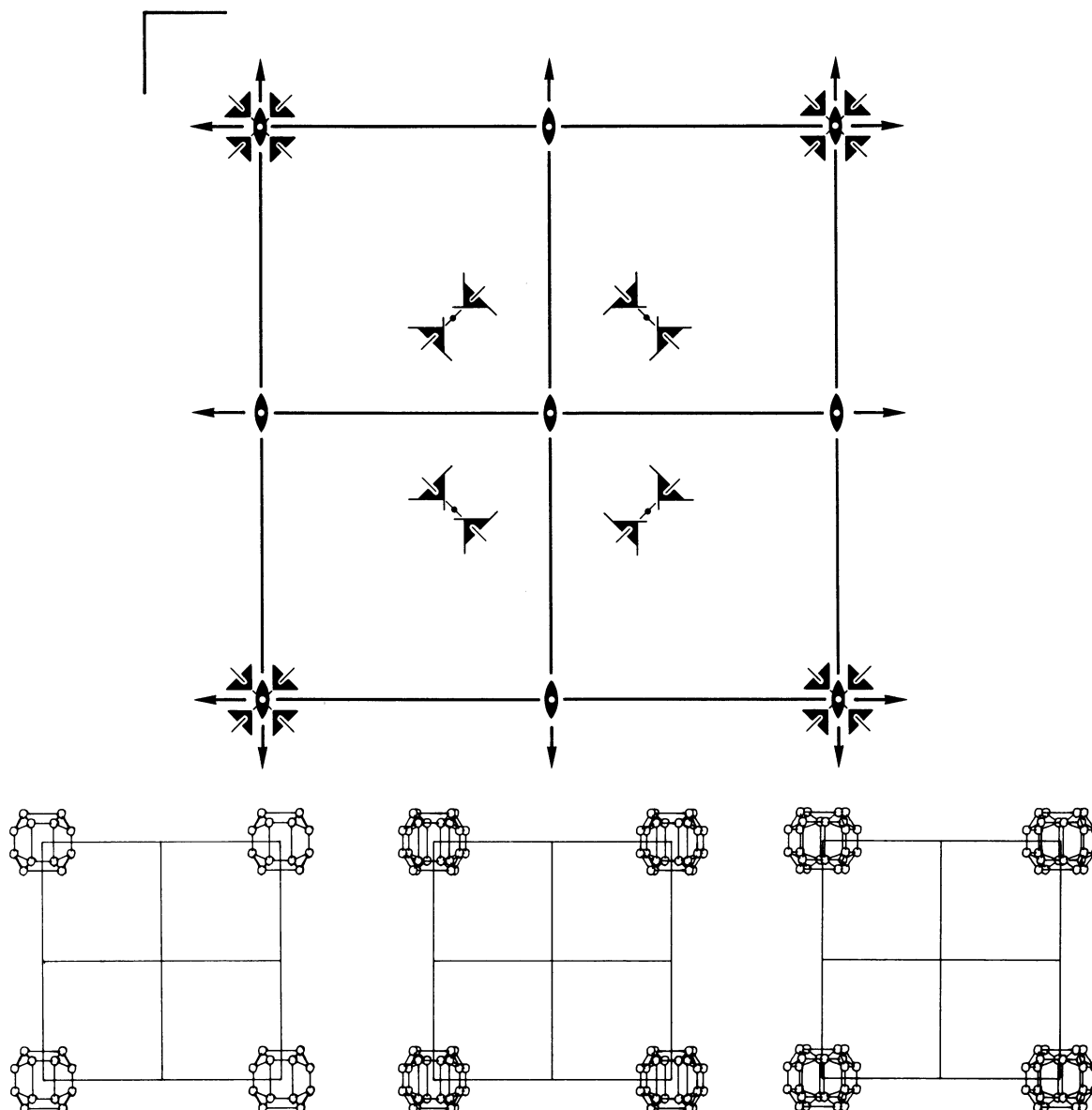
$m\bar{3}$

Cubic

No. 200

$P2/m\bar{3}$

Patterson symmetry $Pm\bar{3}$



Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; z \leq \min(x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------------------------|---|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) 3^+ x, x, x | (6) 3^+ \bar{x}, x, \bar{x} | (7) 3^+ x, \bar{x}, \bar{x} | (8) 3^+ \bar{x}, \bar{x}, x |
| (9) 3^- x, x, x | (10) 3^- x, \bar{x}, \bar{x} | (11) 3^- \bar{x}, \bar{x}, x | (12) 3^- \bar{x}, x, \bar{x} |
| (13) $\bar{1}$ $0, 0, 0$ | (14) m $x, y, 0$ | (15) m $x, 0, z$ | (16) m $0, y, z$ |
| (17) $\bar{3}^+$ $x, x, x; 0, 0, 0$ | (18) $\bar{3}^+$ $\bar{x}, x, \bar{x}; 0, 0, 0$ | (19) $\bar{3}^+$ $x, \bar{x}, \bar{x}; 0, 0, 0$ | (20) $\bar{3}^+$ $\bar{x}, \bar{x}, x; 0, 0, 0$ |
| (21) $\bar{3}^-$ $x, x, x; 0, 0, 0$ | (22) $\bar{3}^-$ $x, \bar{x}, \bar{x}; 0, 0, 0$ | (23) $\bar{3}^-$ $\bar{x}, \bar{x}, x; 0, 0, 0$ | (24) $\bar{3}^-$ $\bar{x}, x, \bar{x}; 0, 0, 0$ |

Minimal non-isomorphic supergroups

I $[2]Pm\bar{3}m(221); [2]Pm\bar{3}n(223)$

II $[2]Im\bar{3}(204); [4]Fm\bar{3}(202)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

 h, k, l cyclically permutable

General:

24	l	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) z, x, y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}
			(9) y, z, x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x
			(13) $\bar{x}, \bar{y}, \bar{z}$	(14) x, y, \bar{z}	(15) x, \bar{y}, z	(16) \bar{x}, y, z
			(17) $\bar{z}, \bar{x}, \bar{y}$	(18) \bar{z}, x, y	(19) z, x, \bar{y}	(20) z, \bar{x}, y
			(21) $\bar{y}, \bar{z}, \bar{x}$	(22) y, \bar{z}, x	(23) \bar{y}, z, x	(24) y, z, \bar{x}

no conditions

Special: no extra conditions

12	k	$m..$	$\frac{1}{2}, y, z$ $\bar{z}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, z$ $\bar{z}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{z}$ $y, z, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{z}$ $\bar{y}, z, \frac{1}{2}$	$z, \frac{1}{2}, y$ $y, \bar{z}, \frac{1}{2}$	$z, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{z}, \frac{1}{2}$
12	j	$m..$	$0, y, z$ $\bar{z}, 0, y$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$	$0, y, \bar{z}$ $y, z, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$	$z, 0, y$ $y, \bar{z}, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$
8	i	$.3.$	x, x, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, \bar{x}, x x, x, \bar{x}	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x		
6	h	$mm2..$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
6	g	$mm2..$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$
6	f	$mm2..$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$0, \frac{1}{2}, x$	$0, \frac{1}{2}, \bar{x}$
6	e	$mm2..$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
3	d	$mmm..$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$			
3	c	$mmm..$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
1	b	$m\bar{3}.$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
1	a	$m\bar{3}.$	$0, 0, 0$					

Symmetry of special projectionsAlong [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [111] $p6$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$ **Maximal non-isomorphic subgroups**

I	[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pm1$ ($Pmmm$, 47)	1; 2; 3; 4; 13; 14; 15; 16
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 5; 9; 13; 17; 21
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 6; 12; 13; 18; 24
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 7; 10; 13; 19; 22
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 8; 11; 13; 20; 23

IIa none**IIb** [2] $Fm\bar{3}$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (202); [4] $Ia\bar{3}$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (206); [4] $Im\bar{3}$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (204)**Maximal isomorphic subgroups of lowest index****IIc** [27] $Pm\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (200)

(Continued on preceding page)

$Pn\bar{3}$

T_h^2

$m\bar{3}$

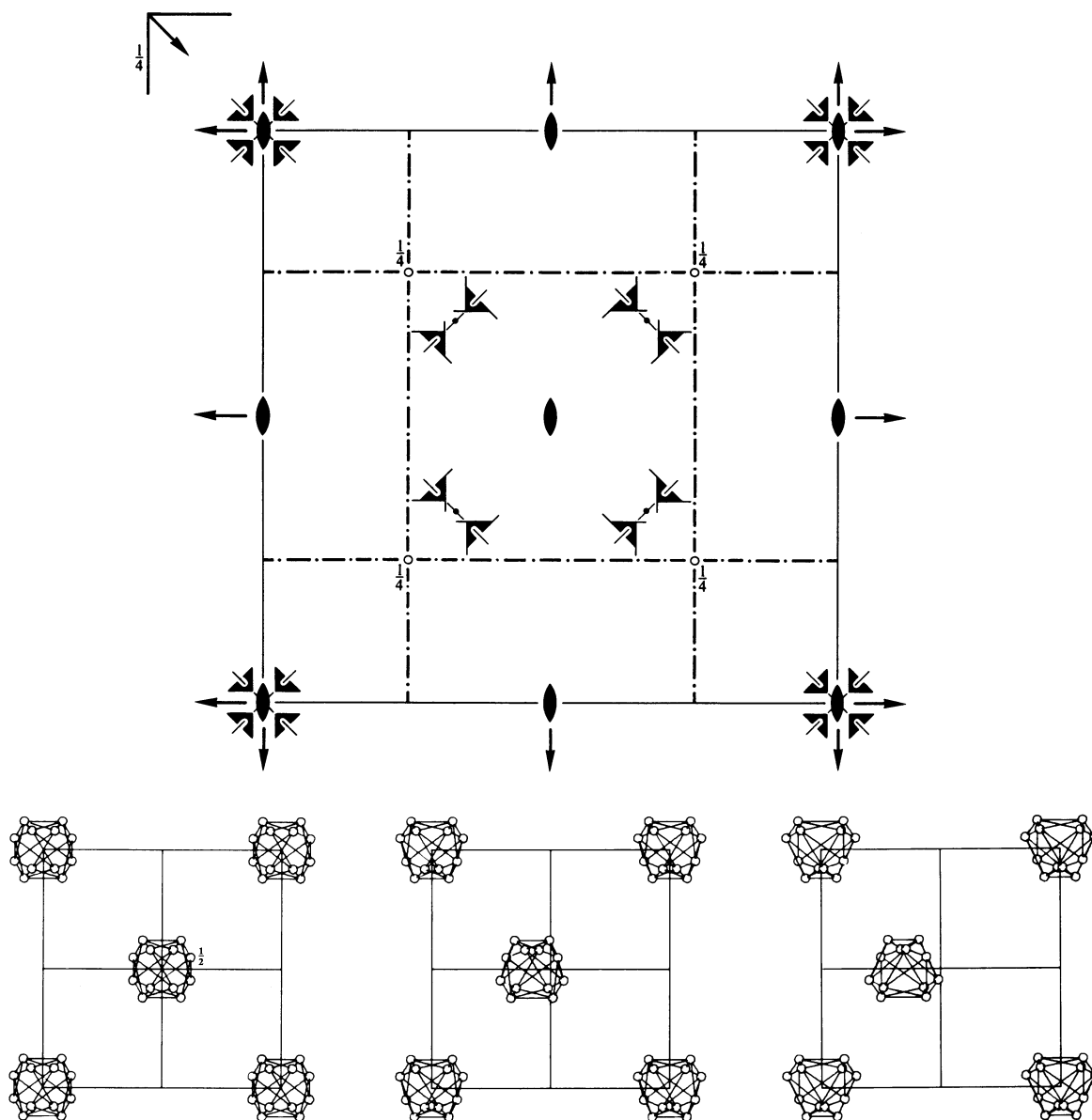
Cubic

No. 201

$P2/n\bar{3}$

Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 1



Origin at 23, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \min(x, 1-x); z \leq y$

Vertices $0, 0, 0 \quad 1, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | | |
|---|--|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) 3^+ x, x, x | (6) 3^+ \bar{x}, x, \bar{x} | (7) 3^+ x, \bar{x}, \bar{x} | (8) 3^+ \bar{x}, \bar{x}, x |
| (9) 3^- x, x, x | (10) 3^- x, \bar{x}, \bar{x} | (11) 3^- \bar{x}, \bar{x}, x | (12) 3^- \bar{x}, x, \bar{x} |
| (13) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (14) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (15) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (16) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |
| (17) $\bar{3}^+$ $x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (18) $\bar{3}^+$ $\bar{x}-1, x+1, \bar{x}; -\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ | (19) $\bar{3}^+$ $x, \bar{x}+1, \bar{x}; \frac{1}{4}, \frac{3}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+$ $\bar{x}+1, \bar{x}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{4}$ |
| (21) $\bar{3}^-$ $x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (22) $\bar{3}^-$ $x+1, \bar{x}-1, \bar{x}; \frac{1}{4}, -\frac{1}{4}, \frac{3}{4}$ | (23) $\bar{3}^-$ $\bar{x}, \bar{x}+1, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ | (24) $\bar{3}^-$ $\bar{x}+1, x, \bar{x}; \frac{3}{4}, \frac{1}{4}, -\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		h, k, l cyclically permutable General:
24 <i>h</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{x}, y, \bar{z} (4) x, \bar{y}, \bar{z} (5) z, x, y (6) z, \bar{x}, \bar{y} (7) \bar{z}, \bar{x}, y (8) \bar{z}, x, \bar{y} (9) y, z, x (10) \bar{y}, z, \bar{x} (11) y, \bar{z}, \bar{x} (12) \bar{y}, \bar{z}, x (13) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (16) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (17) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (18) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}$ (19) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (20) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (21) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (22) $y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (23) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (24) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0kl : k + l = 2n$ $h00 : h = 2n$
		Special: as above, plus
12 <i>g</i> 2..	$x, \frac{1}{2}, 0$ $\bar{x}, \frac{1}{2}, 0$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, 0, x$ $\frac{1}{2}, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $0, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
12 <i>f</i> 2..	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $0, 0, x$ $0, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
8 <i>e</i> .3.	x, x, x \bar{x}, \bar{x}, x \bar{x}, x, \bar{x} x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions
6 <i>d</i> 222..	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $0, 0, \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>c</i> . $\bar{3}$.	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>b</i> . $\bar{3}$.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
2 <i>a</i> 23.	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001] c2mm$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at $0, 0, z$

Along $[111] p6$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110] p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pn1$ ($Pnnn$, 48)	1; 2; 3; 4; 13; 14; 15; 16
	$\left\{ \begin{array}{l} [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \end{array} \right.$	1; 5; 9; 13; 17; 21
		1; 6; 12; 13; 18; 24
		1; 7; 10; 13; 19; 22
		1; 8; 11; 13; 20; 23

IIa none

IIb [2] $Fd\bar{3}$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (203)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (201)

Minimal non-isomorphic supergroups

I [2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

II [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

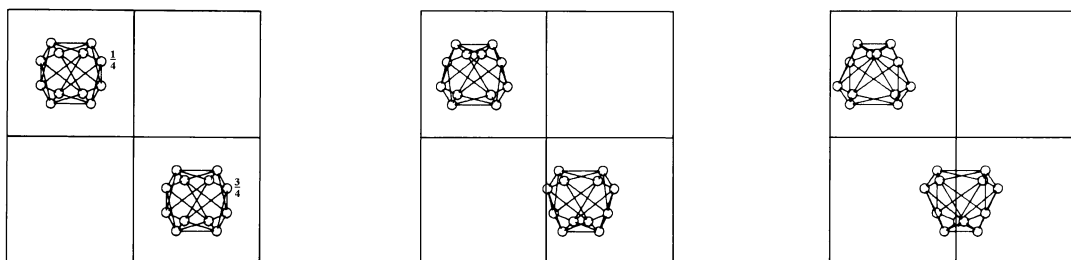
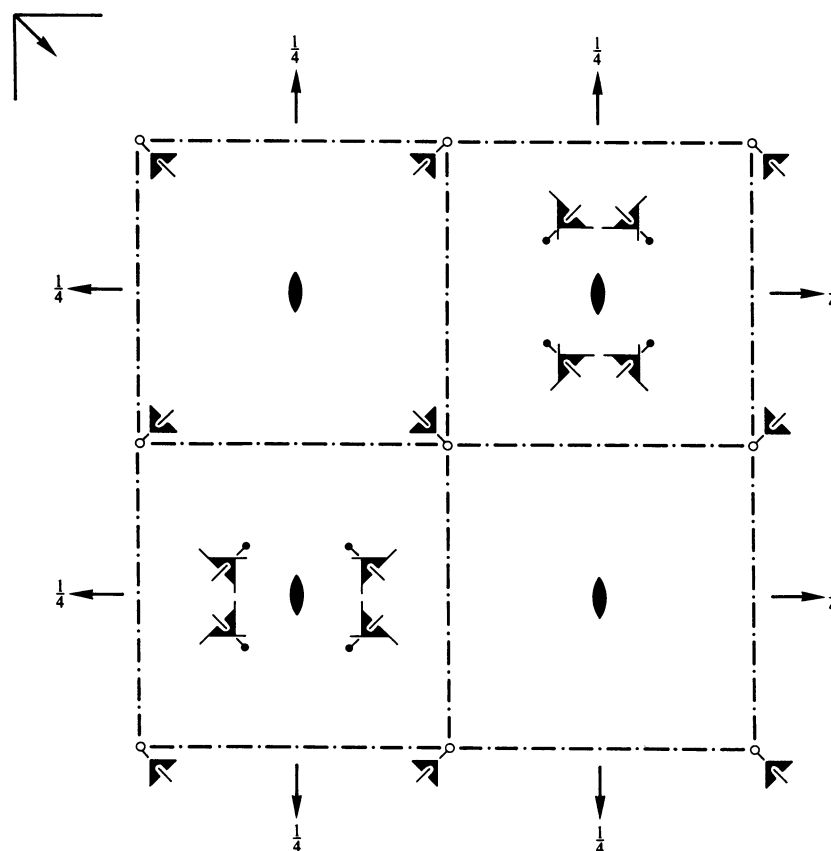
$Pn\bar{3}$ T_h^2 $m\bar{3}$

Cubic

No. 201

 $P2/n\bar{3}$ Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 2

**Origin** at centre ($\bar{3}$), at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from 23**Asymmetric unit** $-\frac{1}{4} \leq x \leq \frac{3}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq \min(x, \frac{1}{2} - x); z \leq y$ Vertices $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}; \frac{3}{4}, -\frac{1}{4}, -\frac{1}{4}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ **Symmetry operations**

- | | | | |
|-------------------------------------|--|--|--|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2 $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) 3^+ x, x, x | (6) 3^+ $\bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) 3^+ $x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) 3^+ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) 3^- x, x, x | (10) 3^- $x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) 3^- $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) 3^- $\bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $\bar{1}$ 0,0,0 | (14) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (15) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (16) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ |
| (17) $\bar{3}^+$ $x, x, x; 0, 0, 0$ | (18) $\bar{3}^+$ $\bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{2}, 0, \frac{1}{2}$ | (19) $\bar{3}^+$ $x - \frac{1}{2}, \bar{x} + 1, \bar{x}; 0, \frac{1}{2}, -\frac{1}{2}$ | (20) $\bar{3}^+$ $\bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \frac{1}{2}, -\frac{1}{2}, 0$ |
| (21) $\bar{3}^-$ $x, x, x; 0, 0, 0$ | (22) $\bar{3}^-$ $x + \frac{1}{2}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{2}, \frac{1}{2}$ | (23) $\bar{3}^-$ $\bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; -\frac{1}{2}, \frac{1}{2}, 0$ | (24) $\bar{3}^-$ $\bar{x} + 1, x - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, -\frac{1}{2}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		h, k, l cyclically permutable General:
24 h 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (5) z, x, y (6) $z, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, y$ (8) $\bar{z} + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (9) y, z, x (10) $\bar{y} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$ (11) $y, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$ (13) $\bar{x}, \bar{y}, \bar{z}$ (14) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (15) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (16) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (17) $\bar{z}, \bar{x}, \bar{y}$ (18) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$ (19) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$ (20) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (21) $\bar{y}, \bar{z}, \bar{x}$ (22) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (23) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$ (24) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	$0kl : k + l = 2n$ $h00 : h = 2n$
		Special: as above, plus
12 g 2..	$x, \frac{3}{4}, \frac{1}{4}$ $\bar{x}, \frac{1}{4}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, x, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{3}{4}, \bar{x}$ $\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
12 f 2..	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$ $\frac{1}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
8 e .3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions
6 d 222..	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4 c . $\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
4 b . $\bar{3}$.	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
2 a 23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [111] $p6$

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$

Origin at x, x, x

Along [110] $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pn1$ ($Pnnn$, 48)	1; 2; 3; 4; 13; 14; 15; 16
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 5; 9; 13; 17; 21
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 6; 12; 13; 18; 24
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 7; 10; 13; 19; 22
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 8; 11; 13; 20; 23

IIa none

IIb [2] $Fd\bar{3}$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (203)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (201)

Minimal non-isomorphic supergroups

I [2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

II [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

$Fm\bar{3}$

T_h^3

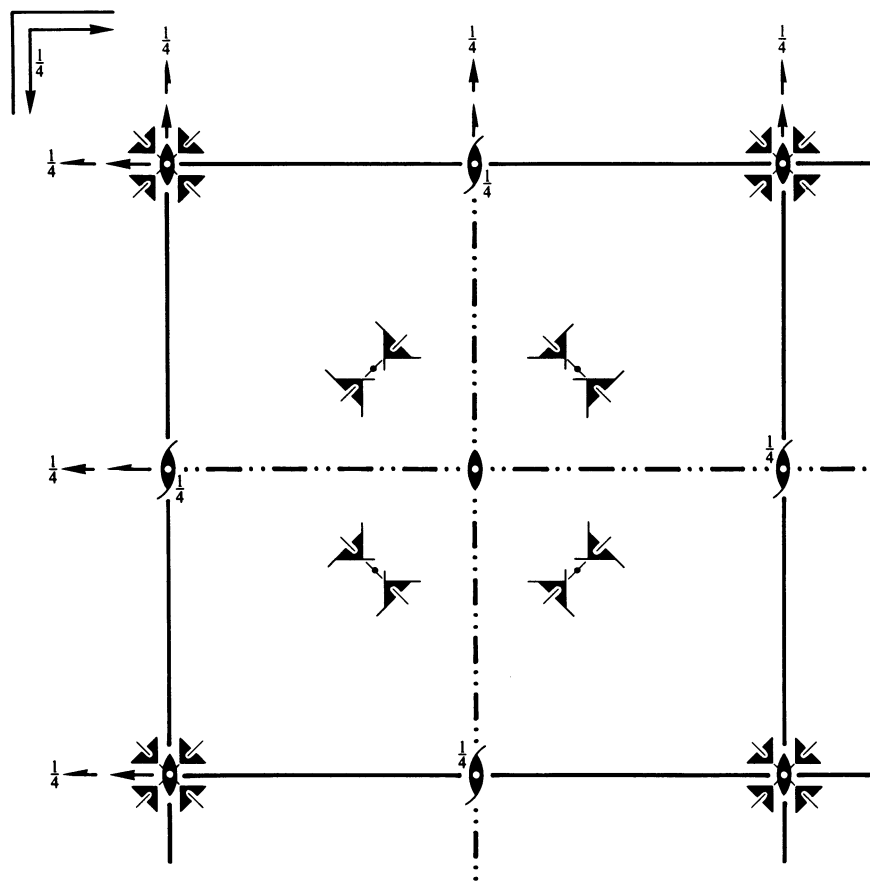
$m\bar{3}$

Cubic

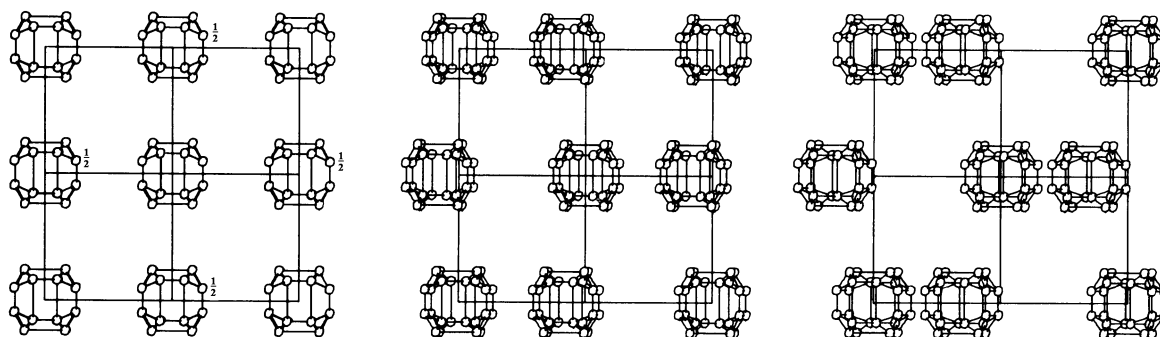
No. 202

$F2/m\bar{3}$

Patterson symmetry $Fm\bar{3}$



Upper left quadrant only



Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$; $y \leq x$; $z \leq \min(\frac{1}{2} - x, y)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|---------------------------------|---|---|---|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) 3^+ x,x,x | (6) 3^+ \bar{x},x,\bar{x} | (7) 3^+ x,\bar{x},\bar{x} | (8) 3^+ \bar{x},\bar{x},x |
| (9) 3^- x,x,x | (10) 3^- x,\bar{x},\bar{x} | (11) 3^- \bar{x},\bar{x},x | (12) 3^- \bar{x},x,\bar{x} |
| (13) $\bar{1}$ $0,0,0$ | (14) m $x,y,0$ | (15) m $x,0,z$ | (16) m $0,y,z$ |
| (17) $\bar{3}^+$ $x,x,x; 0,0,0$ | (18) $\bar{3}^+$ $\bar{x},x,\bar{x}; 0,0,0$ | (19) $\bar{3}^+$ $x,\bar{x},\bar{x}; 0,0,0$ | (20) $\bar{3}^+$ $\bar{x},\bar{x},x; 0,0,0$ |
| (21) $\bar{3}^-$ $x,x,x; 0,0,0$ | (22) $\bar{3}^-$ $x,\bar{x},\bar{x}; 0,0,0$ | (23) $\bar{3}^-$ $\bar{x},\bar{x},x; 0,0,0$ | (24) $\bar{3}^-$ $\bar{x},x,\bar{x}; 0,0,0$ |

Symmetry operations (continued)For $(0, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|--|---|---|---|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2})$ $0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) 2 $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{3}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $\bar{1}$ $0, \frac{1}{4}, \frac{1}{4}$ | (14) b $x, y, \frac{1}{4}$ | (15) c $x, \frac{1}{4}, z$ | (16) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$ |
| (17) $\bar{3}^+$ $x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (18) $\bar{3}^+ \bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{2}, 0, \frac{1}{2}$ | (19) $\bar{3}^+ x, \bar{x} + \frac{1}{2}, \bar{x}; 0, \frac{1}{2}, 0$ | (20) $\bar{3}^+ \bar{x} + 1, \bar{x} + \frac{1}{2}, x; \frac{1}{2}, 0, \frac{1}{2}$ |
| (21) $\bar{3}^-$ $x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (22) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; 0, 0, \frac{1}{2}$ | (23) $\bar{3}^- \bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; -\frac{1}{2}, \frac{1}{2}, 0$ | (24) $\bar{3}^- \bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}; \frac{1}{2}, \frac{1}{2}, 0$ |

For $(\frac{1}{2}, 0, \frac{1}{2})^+$ set

- | | | | |
|--|---|---|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} + \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x - \frac{1}{6}, x - \frac{1}{3}, x$ | (10) $3^- x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) $3^-(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $\bar{1}$ $\frac{1}{4}, 0, \frac{1}{4}$ | (14) a $x, y, \frac{1}{4}$ | (15) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$ | (16) c $\frac{1}{4}, y, z$ |
| (17) $\bar{3}^+$ $x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (18) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}; 0, 0, \frac{1}{2}$ | (19) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \frac{1}{2}, \frac{1}{2}, 0$ | (20) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \frac{1}{2}, -\frac{1}{2}, 0$ |
| (21) $\bar{3}^-$ $x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (22) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{2}, \frac{1}{2}$ | (23) $\bar{3}^- \bar{x} + \frac{1}{2}, \bar{x} + 1, x; 0, \frac{1}{2}, \frac{1}{2}$ | (24) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{2}, 0, 0$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)^+$ set

- | | | | |
|--|---|--|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, x + \frac{1}{3}, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{3}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^- x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^-(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (14) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (15) a $x, \frac{1}{4}, z$ | (16) b $\frac{1}{4}, y, z$ |
| (17) $\bar{3}^+$ $x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (18) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + 1, \bar{x}; 0, \frac{1}{2}, \frac{1}{2}$ | (19) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + 1, \bar{x}; 0, \frac{1}{2}, -\frac{1}{2}$ | (20) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x}, x; \frac{1}{2}, 0, 0$ |
| (21) $\bar{3}^-$ $x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (22) $\bar{3}^- x + 1, \bar{x} - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, \frac{1}{2}$ | (23) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (24) $\bar{3}^- \bar{x} + 1, x - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, -\frac{1}{2}$ |

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)**Positions**

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0, 0, 0)^+$ $(0, \frac{1}{2}, \frac{1}{2})^+$ $(\frac{1}{2}, 0, \frac{1}{2})^+$ $(\frac{1}{2}, \frac{1}{2}, 0)^+$

Reflection conditions

h, k, l cyclically permutable
General:

96	i	1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $\bar{x}, \bar{y}, \bar{z}$ (17) $\bar{z}, \bar{x}, \bar{y}$ (21) $\bar{y}, \bar{z}, \bar{x}$	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) x, y, \bar{z} (18) \bar{z}, x, y (22) y, \bar{z}, x	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) x, \bar{y}, z (19) z, x, \bar{y} (23) \bar{y}, z, x	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{x}, y, z (20) z, \bar{x}, y (24) y, z, \bar{x}	$hkl : h + k, h + l, k + l = 2n$ $0kl : k, l = 2n$ $hhl : h + l = 2n$ $h00 : h = 2n$		
48	h	$m..$	$0, y, z$ $\bar{z}, 0, y$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$	$0, y, \bar{z}$ $y, z, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$	$z, 0, y$ $y, \bar{z}, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$	no extra conditions
48	g	$2..$	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x$	$hkl : h = 2n$
32	f	$.3.$	x, x, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, \bar{x}, x x, x, \bar{x}	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x			no extra conditions
24	e	$mm2..$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions
24	d	$2/m..$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h = 2n$
8	c	$23.$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$					$hkl : h = 2n$
4	b	$m\bar{3}.$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						no extra conditions
4	a	$m\bar{3}.$	$0, 0, 0$						no extra conditions

Symmetry of special projections

Along $[001] p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[111] p6$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110] c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Fm1$ ($Fmmm$, 69)	(1; 2; 3; 4; 13; 14; 15; 16)+
{	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
{	IIa [4] $Pa\bar{3}$ (205)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(0, \frac{1}{2}, \frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 5; 9; 13; 17; 21; (3; 8; 10; 15; 20; 22) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 7; 10; 13; 19; 22; (3; 6; 9; 15; 18; 21) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 8; 11; 13; 20; 23; (3; 5; 12; 15; 17; 24) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pa\bar{3}$ (205)	1; 6; 12; 13; 18; 24; (3; 7; 11; 15; 19; 23) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2}, 0, \frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pn\bar{3}$ (201)	1; 5; 9; 13; 17; 21; (4; 6; 11; 16; 18; 23) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pn\bar{3}$ (201)	1; 7; 10; 13; 19; 22; (4; 8; 12; 16; 20; 24) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pn\bar{3}$ (201)	1; 8; 11; 13; 20; 23; (4; 7; 9; 16; 19; 21) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pn\bar{3}$ (201)	1; 6; 12; 13; 18; 24; (4; 5; 10; 16; 17; 22) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(0, \frac{1}{2}, \frac{1}{2})$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, 0)$
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(\frac{1}{2}, 0, \frac{1}{2})$; (9; 10; 11; 12; 21; 22; 23; 24) + $(0, \frac{1}{2}, \frac{1}{2})$
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$
IIIb	none	

Maximal isomorphic subgroups of lowest index

IIIc [27] $Fm\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (202)

Minimal non-isomorphic supergroups

I [2] $Fm\bar{3}m$ (225); [2] $Fm\bar{3}c$ (226)

II [2] $Pm\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (200)

$Fd\bar{3}$

T_h^4

$m\bar{3}$

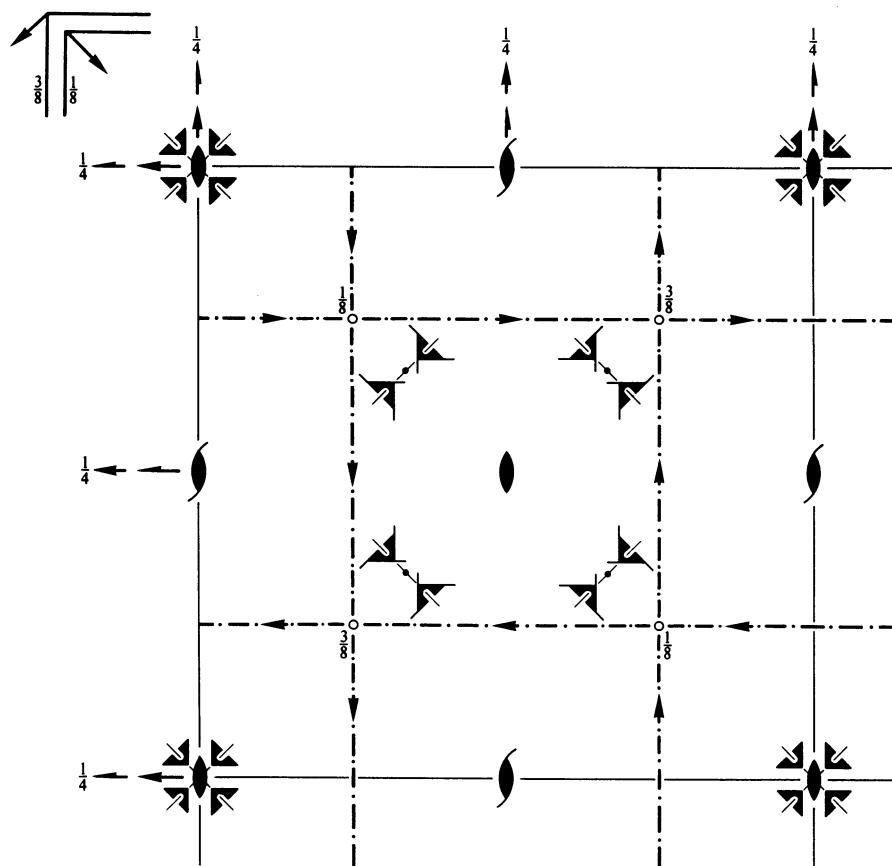
Cubic

No. 203

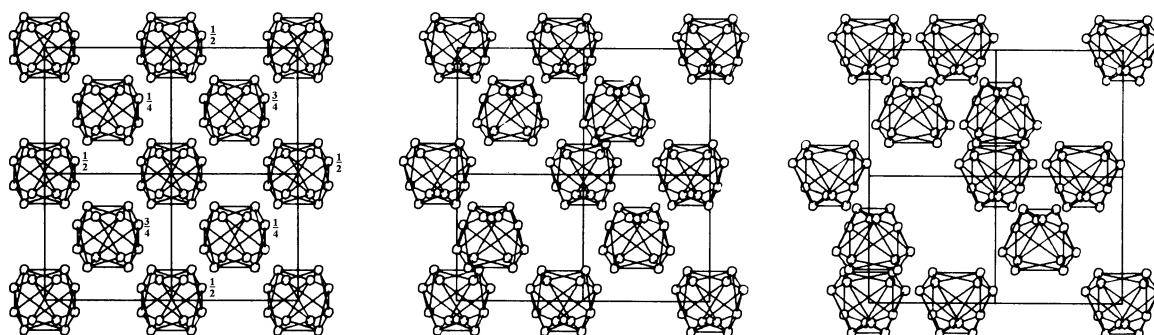
$F2/d\bar{3}$

Patterson symmetry $Fm\bar{3}$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at $2\bar{3}$, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq \min(x, \frac{1}{2} - x); -y \leq z \leq y$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--|--|--|--|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) $\bar{1}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (14) $d(\frac{1}{4}, \frac{1}{4}, 0)$ x,y, $\frac{1}{8}$ | (15) $d(\frac{1}{4}, 0, \frac{1}{4})$ x, $\frac{1}{8},z$ | (16) $d(0, \frac{1}{4}, \frac{1}{4})$ $\frac{1}{8},y,z$ |
| (17) 3 ⁺ x,x,x; $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (18) 3 ⁺ $\bar{x}-\frac{1}{2}, x+\frac{1}{2}, \bar{x}$; $-\frac{1}{8}, \frac{1}{8}, \frac{3}{8}$ | (19) 3 ⁺ x, $\bar{x}+\frac{1}{2}, \bar{x}$; $\frac{1}{8}, \frac{3}{8}, -\frac{1}{8}$ | (20) 3 ⁺ $\bar{x}+\frac{1}{2}, \bar{x}, x$; $\frac{3}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (21) 3 ⁻ x,x,x; $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (22) 3 ⁻ $x+\frac{1}{2}, \bar{x}-\frac{1}{2}, \bar{x}$; $\frac{1}{8}, -\frac{1}{8}, \frac{3}{8}$ | (23) 3 ⁻ $\bar{x}, \bar{x}+\frac{1}{2}, x$; $-\frac{1}{8}, \frac{3}{8}, \frac{1}{8}$ | (24) 3 ⁻ $\bar{x}+\frac{1}{2}, x, \bar{x}$; $\frac{3}{8}, \frac{1}{8}, -\frac{1}{8}$ |

For (0, $\frac{1}{2}$, $\frac{1}{2}$) + set

- | | | | |
|--|--|---|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) 0, $\frac{1}{4},z$ | (3) 2(0, $\frac{1}{2}$,0) 0,y, $\frac{1}{4}$ | (4) 2 x, $\frac{1}{4},\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x-\frac{1}{3}, x-\frac{1}{6}, x$ | (6) 3 ⁺ $\bar{x}, x+\frac{1}{2}, \bar{x}$ | (7) 3 ⁺ ($-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x+\frac{1}{3}, \bar{x}-\frac{1}{6}, \bar{x}$ | (8) 3 ⁺ $\bar{x}, \bar{x}+\frac{1}{2}, x$ |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x-\frac{1}{6}, x+\frac{1}{6}, x$ | (10) 3 ⁻ ($-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x+\frac{1}{6}, \bar{x}+\frac{1}{6}, \bar{x}$ | (11) 3 ⁻ $\bar{x}+\frac{1}{2}, \bar{x}+\frac{1}{2}, x$ | (12) 3 ⁻ $\bar{x}-\frac{1}{2}, x+\frac{1}{2}, \bar{x}$ |
| (13) $\bar{1}$ $\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$ | (14) $d(\frac{1}{4}, \frac{3}{4}, 0)$ x,y, $\frac{3}{8}$ | (15) $d(\frac{1}{4}, 0, \frac{3}{4})$ x, $\frac{3}{8},z$ | (16) $d(0, \frac{3}{4}, \frac{3}{4})$ $\frac{1}{8},y,z$ |
| (17) 3 ⁺ x,x,x; $\frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ | (18) 3 ⁺ $\bar{x}-\frac{3}{2}, x+1, \bar{x}$; $-\frac{5}{8}, \frac{1}{8}, \frac{7}{8}$ | (19) 3 ⁺ x, $\bar{x}+1, \bar{x}$; $\frac{1}{8}, \frac{7}{8}, -\frac{1}{8}$ | (20) 3 ⁺ $\bar{x}+\frac{3}{2}, \bar{x}+\frac{1}{2}, x$; $\frac{7}{8}, -\frac{1}{8}, \frac{5}{8}$ |
| (21) 3 ⁻ $x-\frac{1}{2}, x-\frac{1}{2}, x$; $\frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (22) 3 ⁻ $x+1, \bar{x}-1, \bar{x}$; $\frac{1}{8}, -\frac{1}{8}, \frac{7}{8}$ | (23) 3 ⁻ $\bar{x}-\frac{1}{2}, \bar{x}+1, x$; $-\frac{5}{8}, \frac{7}{8}, \frac{1}{8}$ | (24) 3 ⁻ $\bar{x}+1, x+\frac{1}{2}, \bar{x}$; $\frac{7}{8}, \frac{5}{8}, -\frac{1}{8}$ |

For ($\frac{1}{2}$, 0, $\frac{1}{2}$) + set

- | | | | |
|--|---|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}, 0, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2($\frac{1}{2}$, 0, 0) x,0, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x+\frac{1}{6}, x-\frac{1}{6}, x$ | (6) 3 ⁺ ($\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$) $\bar{x}+\frac{1}{6}, x+\frac{1}{6}, \bar{x}$ | (7) 3 ⁺ $x+\frac{1}{2}, \bar{x}-\frac{1}{2}, \bar{x}$ | (8) 3 ⁺ $\bar{x}+\frac{1}{2}, \bar{x}+\frac{1}{2}, x$ |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x-\frac{1}{6}, x-\frac{1}{6}, x$ | (10) 3 ⁻ $x+\frac{1}{2}, \bar{x}, \bar{x}$ | (11) 3 ⁻ $\bar{x}+\frac{1}{2}, \bar{x}, x$ | (12) 3 ⁻ ($\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$) $\bar{x}-\frac{1}{6}, x+\frac{1}{3}, \bar{x}$ |
| (13) $\bar{1}$ $\frac{3}{8}, \frac{1}{8}, \frac{3}{8}$ | (14) $d(\frac{3}{4}, \frac{1}{4}, 0)$ x,y, $\frac{3}{8}$ | (15) $d(\frac{3}{4}, 0, \frac{1}{4})$ x, $\frac{1}{8},z$ | (16) $d(0, \frac{1}{4}, \frac{3}{4})$ $\frac{3}{8},y,z$ |
| (17) 3 ⁺ $x-\frac{1}{2}, x-\frac{1}{2}, x$; $\frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (18) 3 ⁺ $\bar{x}-1, x+1, \bar{x}$; $-\frac{1}{8}, \frac{5}{8}, \frac{7}{8}$ | (19) 3 ⁺ $x+\frac{1}{2}, \bar{x}+1, \bar{x}$; $\frac{5}{8}, \frac{7}{8}, -\frac{1}{8}$ | (20) 3 ⁺ $\bar{x}+1, \bar{x}-\frac{1}{2}, x$; $\frac{7}{8}, -\frac{5}{8}, \frac{1}{8}$ |
| (21) 3 ⁻ $x+\frac{1}{2}, x, x$; $\frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ | (22) 3 ⁻ $x+1, \bar{x}-\frac{3}{2}, \bar{x}$; $\frac{1}{8}, -\frac{5}{8}, \frac{7}{8}$ | (23) 3 ⁻ $\bar{x}+\frac{1}{2}, \bar{x}+\frac{3}{2}, x$; $-\frac{1}{8}, \frac{7}{8}, \frac{5}{8}$ | (24) 3 ⁻ $\bar{x}+1, x, \bar{x}$; $\frac{7}{8}, \frac{1}{8}, -\frac{1}{8}$ |

For ($\frac{1}{2}$, $\frac{1}{2}$, 0) + set

- | | | | |
|--|--|--|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}, y, 0$ | (4) 2($\frac{1}{2}$, 0, 0) x, $\frac{1}{4}, 0$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x+\frac{1}{6}, x+\frac{1}{3}, x$ | (6) 3 ⁺ $\bar{x}+\frac{1}{2}, x, \bar{x}$ | (7) 3 ⁺ $x+\frac{1}{2}, \bar{x}, \bar{x}$ | (8) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}$) $\bar{x}+\frac{1}{6}, \bar{x}+\frac{1}{3}, x$ |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) $x+\frac{1}{3}, x+\frac{1}{6}, x$ | (10) 3 ⁻ x, $\bar{x}+\frac{1}{2}, \bar{x}$ | (11) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}$) $\bar{x}+\frac{1}{3}, \bar{x}+\frac{1}{6}, x$ | (12) 3 ⁻ $\bar{x}, x+\frac{1}{2}, \bar{x}$ |
| (13) $\bar{1}$ $\frac{3}{8}, \frac{3}{8}, \frac{1}{8}$ | (14) $d(\frac{3}{4}, \frac{3}{4}, 0)$ x,y, $\frac{1}{8}$ | (15) $d(\frac{3}{4}, 0, \frac{1}{4})$ x, $\frac{3}{8},z$ | (16) $d(0, \frac{3}{4}, \frac{1}{4})$ $\frac{3}{8},y,z$ |
| (17) 3 ⁺ $x+\frac{1}{2}, x, x$; $\frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ | (18) 3 ⁺ $\bar{x}-1, x+\frac{3}{2}, \bar{x}$; $-\frac{1}{8}, \frac{5}{8}, \frac{7}{8}$ | (19) 3 ⁺ $x-\frac{1}{2}, \bar{x}+\frac{3}{2}, \bar{x}$; $\frac{1}{8}, \frac{7}{8}, -\frac{5}{8}$ | (20) 3 ⁺ $\bar{x}+1, \bar{x}, x$; $\frac{7}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (21) 3 ⁻ x,x, $\frac{1}{2}, x$; $\frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ | (22) 3 ⁻ $x+\frac{3}{2}, \bar{x}-1, \bar{x}$; $\frac{5}{8}, -\frac{1}{8}, \frac{7}{8}$ | (23) 3 ⁻ $\bar{x}, \bar{x}+1, x$; $-\frac{1}{8}, \frac{7}{8}, \frac{1}{8}$ | (24) 3 ⁻ $\bar{x}+\frac{3}{2}, x-\frac{1}{2}, \bar{x}$; $\frac{7}{8}, \frac{1}{8}, -\frac{5}{8}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$) +	($\frac{1}{2}$, 0, $\frac{1}{2}$) +	($\frac{1}{2}$, $\frac{1}{2}$, 0) +	h, k, l cyclicly permutable General:	
96 g 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $\bar{x}+\frac{1}{4}, \bar{y}+\frac{1}{4}, \bar{z}+\frac{1}{4}$ (17) $\bar{z}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{y}+\frac{1}{4}$ (21) $\bar{y}+\frac{1}{4}, \bar{z}+\frac{1}{4}, \bar{x}+\frac{1}{4}$	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $x+\frac{1}{4}, y+\frac{1}{4}, \bar{z}+\frac{1}{4}$ (18) $\bar{z}+\frac{1}{4}, x+\frac{1}{4}, y+\frac{1}{4}$ (22) $y+\frac{1}{4}, \bar{z}+\frac{1}{4}, x+\frac{1}{4}$	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) $x+\frac{1}{4}, \bar{y}+\frac{1}{4}, z+\frac{1}{4}$ (19) $z+\frac{1}{4}, x+\frac{1}{4}, \bar{y}+\frac{1}{4}$ (23) $\bar{y}+\frac{1}{4}, z+\frac{1}{4}, x+\frac{1}{4}$	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) $\bar{x}+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$ (20) $z+\frac{1}{4}, \bar{x}+\frac{1}{4}, y+\frac{1}{4}$ (24) $y+\frac{1}{4}, z+\frac{1}{4}, \bar{x}+\frac{1}{4}$	$hkl : h+k=2n$ and $h+l, k+l=2n$ $0kl : k+l=4n$ and $k, l=2n$ $hhl : h+l=2n$ $h00 : h=4n$	
48 f 2..	x,0,0 $\bar{x}+\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, 0, 0$ $x+\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0,x,0 $\frac{1}{4}, \bar{x}+\frac{1}{4}, \frac{1}{4}$	0, $\bar{x}, 0$ $\frac{1}{4}, x+\frac{1}{4}, \frac{1}{4}$	0,0,x $\frac{1}{4}, \frac{1}{4}, \bar{x}+\frac{1}{4}$	0,0, \bar{x} $\frac{1}{4}, \frac{1}{4}, x+\frac{1}{4}$ $hkl : h=2n+1$ or $h+k+l=4n$
32 e .3.	x,x,x $\bar{x}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{x}+\frac{1}{4}$	\bar{x}, \bar{x}, x $x+\frac{1}{4}, x+\frac{1}{4}, \bar{x}+\frac{1}{4}$	\bar{x}, x, \bar{x} $x+\frac{1}{4}, \bar{x}+\frac{1}{4}, x+\frac{1}{4}$	x, \bar{x}, \bar{x} $\bar{x}+\frac{1}{4}, x+\frac{1}{4}, x+\frac{1}{4}$	no extra conditions	
16 d . $\bar{3}$.	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{3}{8}$	} $hkl : h=2n+1$ or $h, k, l=4n+2$ or $h, k, l=4n$	
16 c . $\bar{3}$.	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{7}{8}$		
8 b 23.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	}	}		$hkl : h=2n+1$ or $h+k+l=4n$
8 a 23.	0,0,0	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$				

(Continued on page 623)

ORIGIN CHOICE 1

Symmetry of special projections

Along $[001]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[111]$ $p6$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, \frac{1}{8}$

ORIGIN CHOICE 2

Symmetry of special projections

Along $[001]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{8}, \frac{1}{8}, z$

Along $[111]$ $p6$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

- I** $[2] F 23 (196)$ $(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+$
 $[3] F d 1 (F d d d, 70)$ $(1; 2; 3; 4; 13; 14; 15; 16)+$
 $\left\{ \begin{array}{l} [4] F 1 \bar{3} (R \bar{3}, 148) \quad (1; 5; 9; 13; 17; 21)+ \\ [4] F 1 \bar{3} (R \bar{3}, 148) \quad (1; 6; 12; 13; 18; 24)+ \\ [4] F 1 \bar{3} (R \bar{3}, 148) \quad (1; 7; 10; 13; 19; 22)+ \\ [4] F 1 \bar{3} (R \bar{3}, 148) \quad (1; 8; 11; 13; 20; 23)+ \end{array} \right.$

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[27] F d \bar{3} (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (203)$

Minimal non-isomorphic supergroups

I $[2] F d \bar{3} m (227); [2] F d \bar{3} c (228)$

II $[2] P n \bar{3} (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (201)$

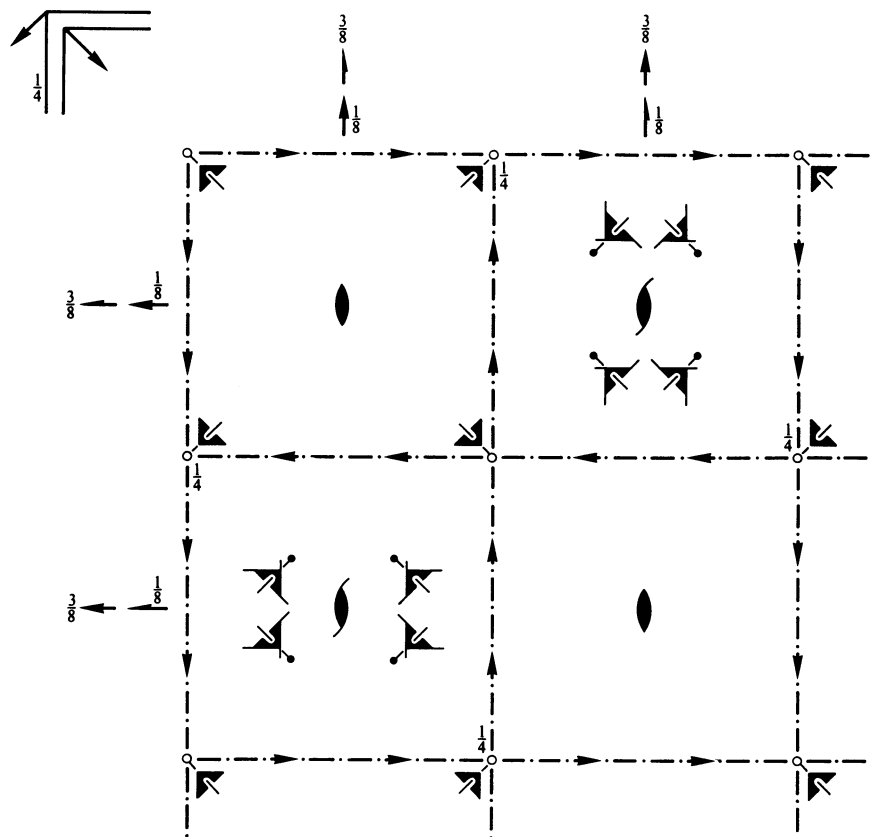
$F d \bar{3}$ T_h^4 $m \bar{3}$

Cubic

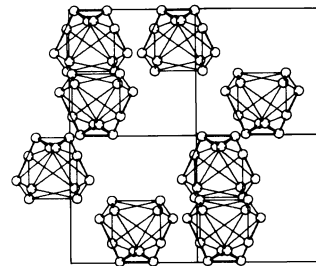
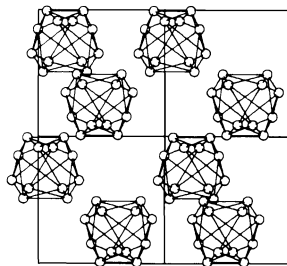
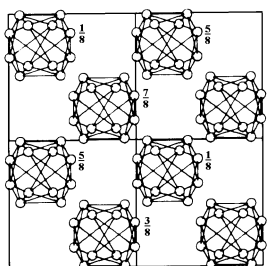
No. 203

 $F 2/d \bar{3}$ Patterson symmetry $F m \bar{3}$

ORIGIN CHOICE 2



Upper left quadrant only

**Origin** at centre ($\bar{3}$), at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 23**Asymmetric unit** $-\frac{1}{8} \leq x \leq \frac{3}{8}; -\frac{1}{8} \leq y \leq \frac{1}{8}; -\frac{3}{8} \leq z \leq \frac{1}{8}; y \leq \min(x, \frac{1}{4} - x); -y - \frac{1}{4} \leq z \leq y$ Vertices $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{3}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-----------------------------------|--|--|--|
| (1) 1 | (2) $2 \frac{3}{8}, \frac{3}{8}, z$ | (3) $2 \frac{3}{8}, y, \frac{3}{8}$ | (4) $2 x, \frac{3}{8}, \frac{3}{8}$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x}, x + \frac{3}{4}, \bar{x}$ | (7) $3^+ x + \frac{3}{4}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- x + \frac{3}{4}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ | (12) $3^- \bar{x}, x + \frac{3}{4}, \bar{x}$ |
| (13) $\bar{1} 0, 0, 0$ | (14) $d(\frac{1}{4}, \frac{1}{4}, 0) x, y, 0$ | (15) $d(\frac{1}{4}, 0, \frac{1}{4}) x, 0, z$ | (16) $d(0, \frac{1}{4}, \frac{1}{4}) 0, y, z$ |
| (17) $\bar{3}^+ x, x, x; 0, 0, 0$ | (18) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{4}, \bar{x}; -\frac{1}{4}, 0, \frac{1}{4}$ | (19) $\bar{3}^+ x - \frac{1}{4}, \bar{x} + \frac{1}{2}, \bar{x}; 0, \frac{1}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+ \bar{x} + \frac{1}{4}, \bar{x} - \frac{1}{4}, x; \frac{1}{4}, -\frac{1}{4}, 0$ |
| (21) $\bar{3}^- x, x, x; 0, 0, 0$ | (22) $\bar{3}^- x + \frac{1}{4}, \bar{x} - \frac{1}{2}, \bar{x}; 0, -\frac{1}{4}, \frac{1}{4}$ | (23) $\bar{3}^- \bar{x} - \frac{1}{4}, \bar{x} + \frac{1}{4}, x; -\frac{1}{4}, \frac{1}{4}, 0$ | (24) $\bar{3}^- \bar{x} + \frac{1}{2}, x - \frac{1}{4}, \bar{x}; \frac{1}{4}, 0, -\frac{1}{4}$ |

For (0, 1/2, 1/2)+ set

- | | | | |
|--|--|--|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \frac{3}{8}, \frac{3}{8}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{3}{8}, y, \frac{1}{8}$ | (4) $2 x, \frac{1}{8}, \frac{1}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{4}, \bar{x}$ | (7) $3^+ x + \frac{3}{4}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \bar{x} + \frac{5}{12}, \bar{x} + \frac{7}{12}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^- x + \frac{1}{4}, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ | (12) $3^-(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \bar{x} - \frac{1}{6}, x + \frac{7}{12}, \bar{x}$ |
| (13) $\bar{1} 0, \frac{1}{4}, \frac{1}{4}$ | (14) $d(\frac{1}{4}, \frac{3}{4}, 0) x, y, \frac{1}{4}$ | (15) $d(\frac{1}{4}, 0, \frac{3}{4}) x, \frac{1}{4}, z$ | (16) $d(0, \frac{3}{4}, \frac{1}{4}) 0, y, z$ |
| (17) $\bar{3}^+ x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (18) $\bar{3}^+ \bar{x} - \frac{3}{2}, x + \frac{3}{4}, \bar{x}; -\frac{3}{4}, 0, \frac{3}{4}$ | (19) $\bar{3}^+ x - \frac{1}{4}, \bar{x} + 1, \bar{x}; 0, \frac{3}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+ \bar{x} + \frac{5}{4}, \bar{x} + \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{2}$ |
| (21) $\bar{3}^- x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (22) $\bar{3}^- x + \frac{3}{4}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{4}, \frac{3}{4}$ | (23) $\bar{3}^- \bar{x} - \frac{3}{4}, \bar{x} + \frac{3}{4}, x; -\frac{3}{4}, \frac{3}{4}, 0$ | (24) $\bar{3}^- \bar{x} + 1, x + \frac{1}{4}, \bar{x}; \frac{3}{4}, \frac{1}{2}, -\frac{1}{4}$ |

For (1/2, 0, 1/2)+ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \frac{1}{8}, \frac{3}{8}, z$ | (3) $2 \frac{1}{8}, y, \frac{1}{8}$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{3}{8}, \frac{1}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x + \frac{1}{4}, \bar{x}$ | (7) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{7}{12}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{6}, x - \frac{1}{3}, x$ | (10) $3^- x + \frac{1}{4}, \bar{x}, \bar{x}$ | (11) $3^-(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \bar{x} + \frac{7}{12}, \bar{x} + \frac{5}{12}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{3}{4}, \bar{x}$ |
| (13) $\bar{1} \frac{1}{4}, 0, \frac{1}{4}$ | (14) $d(\frac{3}{4}, \frac{1}{4}, 0) x, y, \frac{1}{4}$ | (15) $d(\frac{3}{4}, 0, \frac{3}{4}) x, 0, z$ | (16) $d(0, \frac{1}{4}, \frac{3}{4}) \frac{1}{4}, y, z$ |
| (17) $\bar{3}^+ x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (18) $\bar{3}^+ \bar{x} - 1, x + \frac{3}{4}, \bar{x}; -\frac{1}{4}, 0, \frac{3}{4}$ | (19) $\bar{3}^+ x + \frac{1}{4}, \bar{x} + 1, \bar{x}; \frac{1}{2}, \frac{3}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} - \frac{3}{4}, x; \frac{3}{4}, -\frac{3}{4}, 0$ |
| (21) $\bar{3}^- x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (22) $\bar{3}^- x + \frac{3}{4}, \bar{x} - \frac{3}{2}, \bar{x}; 0, -\frac{3}{4}, \frac{3}{4}$ | (23) $\bar{3}^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{5}{4}, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ | (24) $\bar{3}^- \bar{x} + 1, x - \frac{1}{4}, \bar{x}; \frac{3}{4}, 0, -\frac{1}{4}$ |

For (1/2, 1/2, 0)+ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2 \frac{1}{8}, \frac{1}{8}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{1}{8}, y, \frac{3}{8}$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{8}, \frac{3}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x + \frac{1}{3}, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \bar{x} + \frac{1}{6}, x + \frac{5}{12}, \bar{x}$ | (7) $3^+ x + \frac{1}{4}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{5}{12}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x$ | (12) $3^- \bar{x}, x + \frac{1}{4}, \bar{x}$ |
| (13) $\bar{1} \frac{1}{4}, \frac{1}{4}, 0$ | (14) $d(\frac{3}{4}, \frac{3}{4}, 0) x, y, 0$ | (15) $d(\frac{3}{4}, 0, \frac{1}{4}) x, \frac{1}{4}, z$ | (16) $d(0, \frac{3}{4}, \frac{1}{4}) \frac{1}{4}, y, z$ |
| (17) $\bar{3}^+ x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (18) $\bar{3}^+ \bar{x} - 1, x + \frac{5}{4}, \bar{x}; -\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ | (19) $\bar{3}^+ x - \frac{3}{4}, \bar{x} + \frac{3}{2}, \bar{x}; 0, \frac{3}{4}, -\frac{3}{4}$ | (20) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} - \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, 0$ |
| (21) $\bar{3}^- x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (22) $\bar{3}^- x + \frac{5}{4}, \bar{x} - 1, \bar{x}; \frac{1}{2}, -\frac{1}{4}, \frac{3}{4}$ | (23) $\bar{3}^- \bar{x} - \frac{1}{4}, \bar{x} + \frac{3}{4}, x; -\frac{1}{4}, \frac{3}{4}, 0$ | (24) $\bar{3}^- \bar{x} + \frac{3}{2}, x - \frac{3}{4}, \bar{x}; \frac{3}{4}, 0, -\frac{3}{4}$ |

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions		
	(0, 0, 0)+	(0, 1/2, 1/2)+	(1/2, 0, 1/2)+	(1/2, 1/2, 0)+	h, k, l cyclicly permutable General:		
96 g 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $\bar{x}, \bar{y}, \bar{z}$ (17) $\bar{z}, \bar{x}, \bar{y}$ (21) $\bar{y}, \bar{z}, \bar{x}$	(2) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, z$ (6) $z, \bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}$ (10) $\bar{y} + \frac{3}{4}, z, \bar{x} + \frac{3}{4}$ (14) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z}$ (18) $\bar{z}, x + \frac{1}{4}, y + \frac{1}{4}$ (22) $y + \frac{1}{4}, \bar{z}, x + \frac{1}{4}$	(3) $\bar{x} + \frac{3}{4}, y, \bar{z} + \frac{3}{4}$ (7) $\bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}, y$ (11) $y, \bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}$ (15) $x + \frac{1}{4}, \bar{y}, z + \frac{1}{4}$ (19) $z + \frac{1}{4}, x + \frac{1}{4}, \bar{y}$ (23) $\bar{y}, z + \frac{1}{4}, x + \frac{1}{4}$	(4) $x, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (8) $\bar{z} + \frac{3}{4}, x, \bar{y} + \frac{3}{4}$ (12) $\bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}, x$ (16) $\bar{x}, y + \frac{1}{4}, z + \frac{1}{4}$ (20) $z + \frac{1}{4}, \bar{x}, y + \frac{1}{4}$ (24) $y + \frac{1}{4}, z + \frac{1}{4}, \bar{x}$	$hkl : h + k, h + l, k + l = 2n$ $0kl : k + l = 4n, k, l = 2n$ $hhl : h + l = 2n$ $h00 : h = 4n$		
48 f 2..	$x, \frac{1}{8}, \frac{1}{8}$ $\bar{x}, \frac{7}{8}, \frac{7}{8}$	$\bar{x} + \frac{3}{4}, \frac{5}{8}, \frac{1}{8}$ $x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}$	$\frac{1}{8}, x, \frac{1}{8}$ $\frac{7}{8}, \bar{x}, \frac{7}{8}$	$\frac{1}{8}, \bar{x} + \frac{3}{4}, \frac{5}{8}$ $\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}$	$\frac{1}{8}, \frac{1}{8}, x$ $\frac{7}{8}, \frac{7}{8}, \bar{x}$	$\frac{5}{8}, \frac{1}{8}, \bar{x} + \frac{3}{4}$ $\frac{3}{8}, \frac{7}{8}, x + \frac{1}{4}$	$hkl : h = 2n + 1$ or $h + k + l = 4n$
32 e .3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$	$\bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ $x + \frac{1}{4}, x + \frac{1}{4}, \bar{x}$	$\bar{x} + \frac{3}{4}, x, \bar{x} + \frac{3}{4}$ $x + \frac{1}{4}, \bar{x}, x + \frac{1}{4}$	$x, \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}$ $\bar{x}, x + \frac{1}{4}, x + \frac{1}{4}$	no extra conditions		
16 d . $\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$		
16 c . $\bar{3}$.	$0, 0, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{3}{4}$	$0, \frac{3}{4}, \frac{3}{4}$			
8 b 23.	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$		$hkl : h = 2n + 1$ or $h + k + l = 4n$		
8 a 23.	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$					

(Continued on page 623)

ORIGIN CHOICE 1

Symmetry of special projections

Along $[001]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[111]$ $p6$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, \frac{1}{8}$

ORIGIN CHOICE 2

Symmetry of special projections

Along $[001]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{8}, \frac{1}{8}, z$

Along $[111]$ $p6$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

- I** $[2] F 23 (196)$ $(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+$
 $[3] F d1 (F d d d, 70)$ $(1; 2; 3; 4; 13; 14; 15; 16)+$
 $\left\{ \begin{array}{l} [4] F 1\bar{3} (R\bar{3}, 148) \\ [4] F 1\bar{3} (R\bar{3}, 148) \\ [4] F 1\bar{3} (R\bar{3}, 148) \\ [4] F 1\bar{3} (R\bar{3}, 148) \end{array} \right.$ $\begin{array}{l} (1; 5; 9; 13; 17; 21)+ \\ (1; 6; 12; 13; 18; 24)+ \\ (1; 7; 10; 13; 19; 22)+ \\ (1; 8; 11; 13; 20; 23)+ \end{array}$

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[27] F d\bar{3} (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (203)$

Minimal non-isomorphic supergroups

I $[2] F d\bar{3} m (227); [2] F d\bar{3} c (228)$

II $[2] P n\bar{3} (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (201)$

$I\bar{m}\bar{3}$

T_h^5

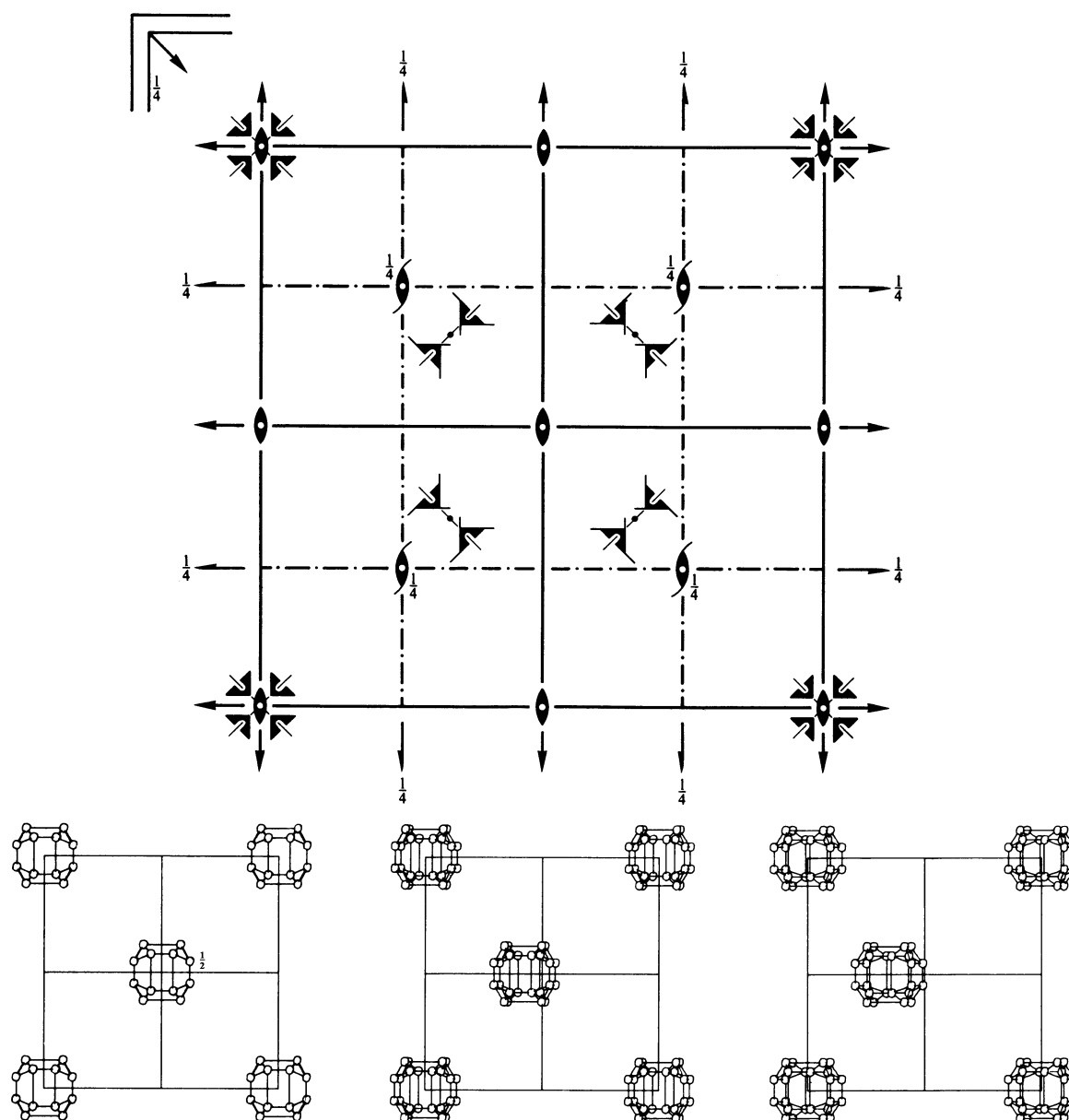
$m\bar{3}$

Cubic

No. 204

$I2/m\bar{3}$

Patterson symmetry $I\bar{m}\bar{3}$



Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $y \leq x$; $z \leq y$
 Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-------------------------------|---|---|--|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3^+ x,x,x | (6) 3^+ \bar{x} ,x, \bar{x} | (7) 3^+ x, \bar{x} , \bar{x} | (8) 3^+ \bar{x} , \bar{x} ,x |
| (9) 3^- x,x,x | (10) 3^- x, \bar{x} , \bar{x} | (11) 3^- \bar{x} , \bar{x} ,x | (12) 3^- \bar{x} ,x, \bar{x} |
| (13) $\bar{1}$ 0,0,0 | (14) m x,y,0 | (15) m x,0,z | (16) m 0,y,z |
| (17) $\bar{3}^+$ x,x,x; 0,0,0 | (18) $\bar{3}^+$ \bar{x} ,x, \bar{x} ; 0,0,0 | (19) $\bar{3}^+$ x, \bar{x} , \bar{x} ; 0,0,0 | (20) $\bar{3}^+$ \bar{x} , \bar{x} ,x; 0,0,0 |
| (21) $\bar{3}^-$ x,x,x; 0,0,0 | (22) $\bar{3}^-$ x, \bar{x} , \bar{x} ; 0,0,0 | (23) $\bar{3}^-$ \bar{x} , \bar{x} ,x; 0,0,0 | (24) $\bar{3}^-$ \bar{x} ,x, \bar{x} ; 0,0,0 |

For ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+ set

- | | | | |
|---|--|--|--|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,x,x | (6) $3^+(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$ | (7) $3^+(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$ | (8) $3^+(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,x,x | (10) $3^-(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$ | (11) $3^-(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6})$ $\bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$ | (12) $3^-(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$ |
| (13) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (14) $n(\frac{1}{2}, \frac{1}{2}, 0)$ x,y, $\frac{1}{4}$ | (15) $n(\frac{1}{2}, 0, \frac{1}{2})$ x, $\frac{1}{4}$,z | (16) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |
| (17) $\bar{3}^+$ x,x,x; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (18) $\bar{3}^+$ $\bar{x} - 1, x + 1, \bar{x}$; $-\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ | (19) $\bar{3}^+$ x, $\bar{x} + 1, \bar{x}$; $\frac{1}{4}, \frac{3}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+$ $\bar{x} + 1, \bar{x}, x$; $\frac{3}{4}, -\frac{1}{4}, \frac{1}{4}$ |
| (21) $\bar{3}^-$ x,x,x; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (22) $\bar{3}^-$ x+1, $\bar{x} - 1, \bar{x}$; $\frac{1}{4}, -\frac{1}{4}, \frac{3}{4}$ | (23) $\bar{3}^-$ $\bar{x}, \bar{x} + 1, x$; $-\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ | (24) $\bar{3}^-$ $\bar{x} + 1, x, \bar{x}$; $\frac{3}{4}, \frac{1}{4}, -\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	h, k, l cyclically permutable General: $hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$
48 <i>h</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{x}, y, \bar{z} (4) x, \bar{y}, \bar{z} (5) z, x, y (6) z, \bar{x}, \bar{y} (7) \bar{z}, \bar{x}, y (8) \bar{z}, x, \bar{y} (9) y, z, x (10) \bar{y}, z, \bar{x} (11) y, \bar{z}, \bar{x} (12) \bar{y}, \bar{z}, x (13) $\bar{x}, \bar{y}, \bar{z}$ (14) x, y, \bar{z} (15) x, \bar{y}, z (16) \bar{x}, y, z (17) $\bar{z}, \bar{x}, \bar{y}$ (18) \bar{z}, x, y (19) z, x, \bar{y} (20) z, \bar{x}, y (21) $\bar{y}, \bar{z}, \bar{x}$ (22) y, \bar{z}, x (23) \bar{y}, z, x (24) y, z, \bar{x}	Special: as above, plus
24 <i>g</i> $m..$	$0, y, z$ $0, \bar{y}, z$ $0, y, \bar{z}$ $0, \bar{y}, \bar{z}$ $z, 0, y$ $z, 0, \bar{y}$ $\bar{z}, 0, y$ $\bar{z}, 0, \bar{y}$ $y, z, 0$ $\bar{y}, z, 0$ $y, \bar{z}, 0$ $\bar{y}, \bar{z}, 0$	no extra conditions
16 <i>f</i> $.3.$	x, x, x \bar{x}, \bar{x}, x \bar{x}, x, \bar{x} x, \bar{x}, \bar{x} $\bar{x}, \bar{x}, \bar{x}$ x, x, \bar{x} x, \bar{x}, x \bar{x}, x, x	no extra conditions
12 <i>e</i> $mm2..$	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $\frac{1}{2}, x, 0$ $\frac{1}{2}, \bar{x}, 0$ $0, \frac{1}{2}, x$ $0, \frac{1}{2}, \bar{x}$	no extra conditions
12 <i>d</i> $mm2..$	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $0, 0, x$ $0, 0, \bar{x}$	no extra conditions
8 <i>c</i> $.\bar{3}.$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : k, l = 2n$
6 <i>b</i> $mmm..$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions
2 <i>a</i> $m\bar{3}.$	$0, 0, 0$	no extra conditions

Symmetry of special projections

Along [001] $c2mm$	Along [111] $p6$	Along [110] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $0, 0, z$	Origin at x, x, x	Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I23$ (197)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Im\bar{1}$ ($Immm$, 71)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
IIa	[2] $Pn\bar{3}$ (201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Im\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (204)

Minimal non-isomorphic supergroups

I	[2] $Im\bar{3}m$ (229)
II	[4] $Pm\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (200)

$Pa\bar{3}$

T_h^6

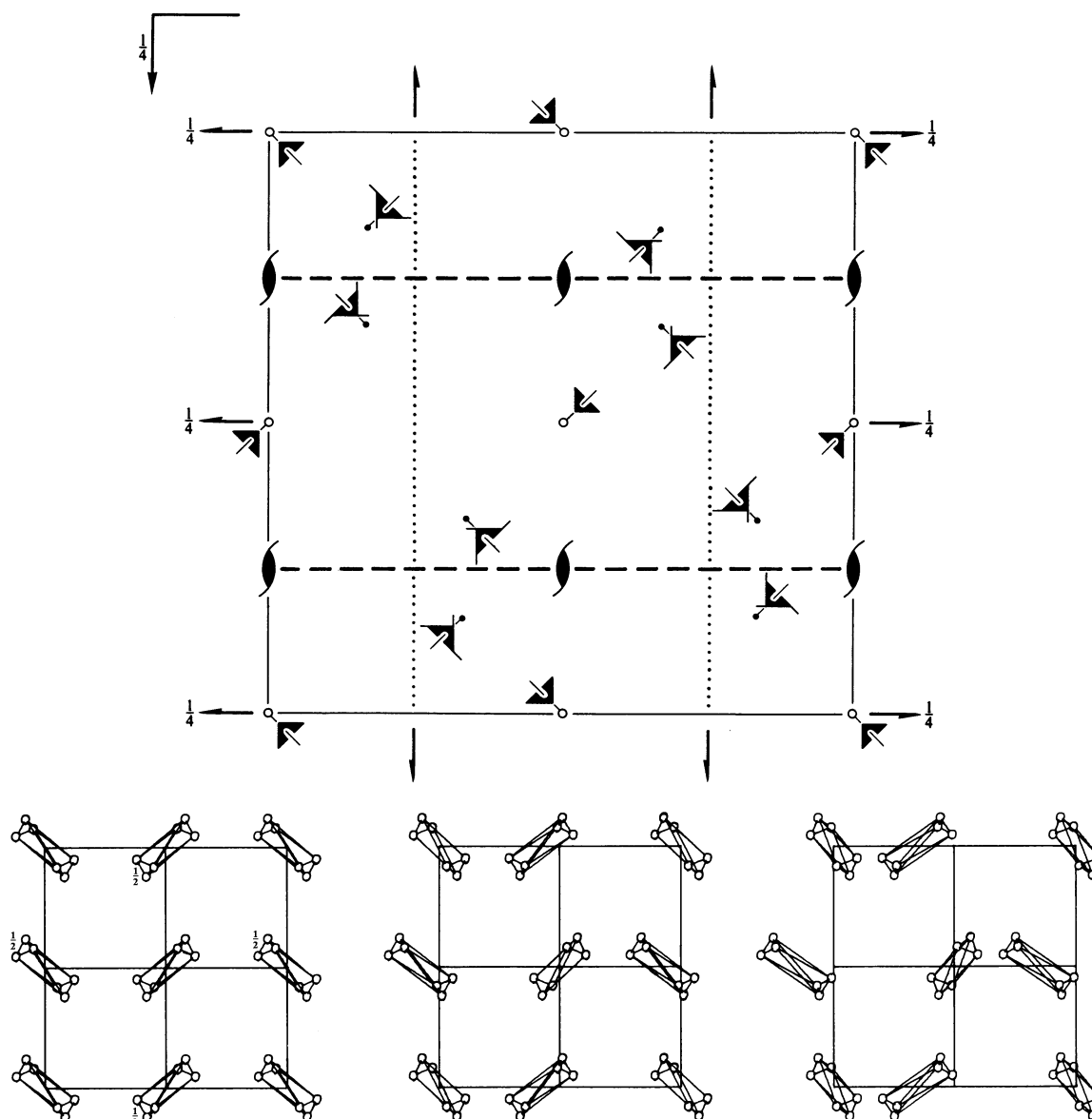
$m\bar{3}$

Cubic

No. 205

$P2_1/a\bar{3}$

Patterson symmetry $Pm\bar{3}$



Origin at centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $z \leq \min(x, y)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | | |
|--|--|---|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) 3^+ x, x, x | (6) 3^+ $\bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) 3^+ $x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) 3^+ $\bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) 3^- x, x, x | (10) $3^-(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^-(-\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^-(-\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $\bar{1}$ $0, 0, 0$ | (14) a $x, y, \frac{1}{4}$ | (15) c $x, \frac{1}{4}, z$ | (16) b $\frac{1}{4}, y, z$ |
| (17) $\bar{3}^+$ x, x, x ; $0, 0, 0$ | (18) $\bar{3}^+$ $\bar{x} - \frac{1}{2}, x + 1, \bar{x}$; $0, \frac{1}{2}, \frac{1}{2}$ | (19) $\bar{3}^+$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$; $\frac{1}{2}, \frac{1}{2}, 0$ | (20) $\bar{3}^+$ $\bar{x} + 1, \bar{x} + \frac{1}{2}, x$; $\frac{1}{2}, 0, \frac{1}{2}$ |
| (21) $\bar{3}^-$ x, x, x ; $0, 0, 0$ | (22) $\bar{3}^-$ $x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$; $0, 0, \frac{1}{2}$ | (23) $\bar{3}^-$ $\bar{x}, \bar{x} + \frac{1}{2}, x$; $0, \frac{1}{2}, 0$ | (24) $\bar{3}^-$ $\bar{x} + \frac{1}{2}, x, \bar{x}$; $\frac{1}{2}, 0, 0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					h, k, l cyclically permutable General:
24 d 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $\bar{x}, \bar{y}, \bar{z}$ (17) $\bar{z}, \bar{x}, \bar{y}$ (21) $\bar{y}, \bar{z}, \bar{x}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$ (10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (14) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (18) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ (22) $y, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$ (15) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (19) $z + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (23) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (16) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (20) $z, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (24) $y + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$	$0kl : k = 2n$ $h00 : h = 2n$
8 c .3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x$	Special: as above, plus no extra conditions
4 b . $\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 a . $\bar{3}$.	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$

Symmetry of special projections

Along $[001]$ $p2gm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at $0, 0, z$

Along $[111]$ $p6$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$$

Origin at x, x, x

$$\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Along $[110]$ $p2gg$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$$

Origin at $x, x, 0$

$$\mathbf{b}' = \mathbf{c}$$

Maximal non-isomorphic subgroups

I	[2] $P2_13$ (198)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pa1$ ($Pbca$, 61)	1; 2; 3; 4; 13; 14; 15; 16
	$\left\{ \begin{array}{l} [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \end{array} \right.$	1; 5; 9; 13; 17; 21
		1; 6; 12; 13; 18; 24
		1; 7; 10; 13; 19; 22
		1; 8; 11; 13; 20; 23

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[27] Pa\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (205)

Minimal non-isomorphic supergroups

I none

II $[2] Ia\bar{3}$ (206); $[4] Fm\bar{3}$ (202)

$Ia\bar{3}$

T_h^7

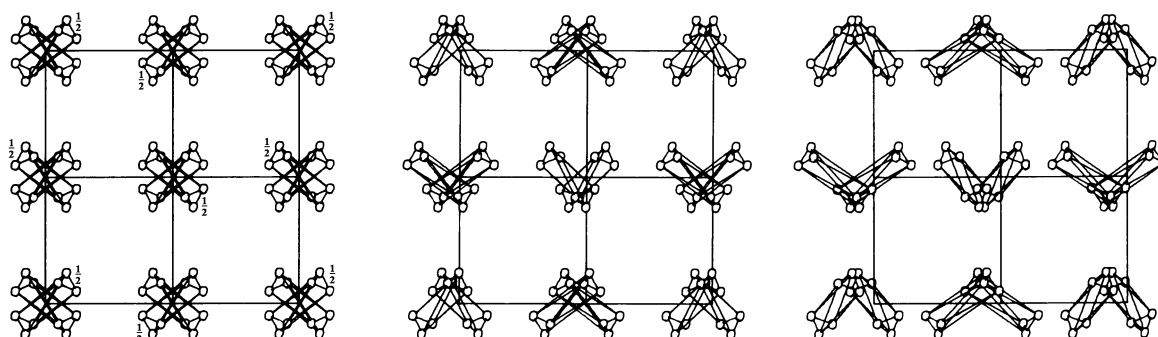
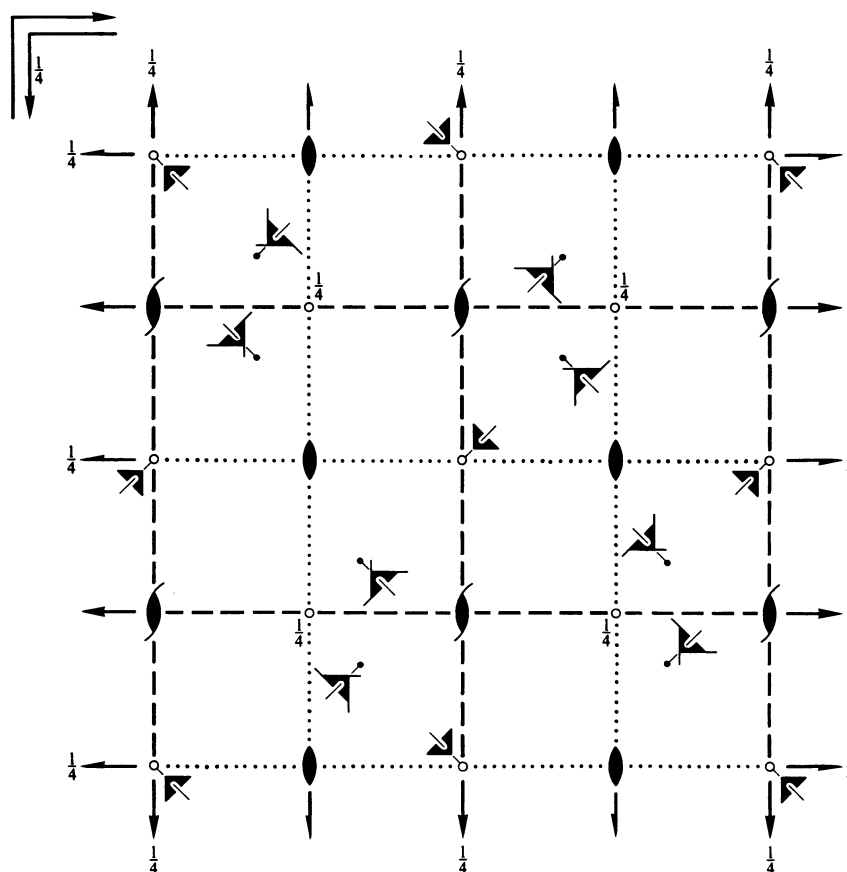
$m\bar{3}$

Cubic

No. 206

$I2_1/a\bar{3}$

Patterson symmetry $Im\bar{3}$



Origin at centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; z \leq \min(x, \frac{1}{2} - x, y, \frac{1}{2} - y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-----------------------------------|---|---|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- (-\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $\bar{1} \quad 0, 0, 0$ | (14) $a \quad x, y, \frac{1}{4}$ | (15) $c \quad x, \frac{1}{4}, z$ | (16) $b \quad \frac{1}{4}, y, z$ |
| (17) $\bar{3}^+ x, x, x; 0, 0, 0$ | (18) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + 1, \bar{x}; 0, \frac{1}{2}, \frac{1}{2}$ | (19) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \frac{1}{2}, \frac{1}{2}, 0$ | (20) $\bar{3}^+ \bar{x} + 1, \bar{x} + \frac{1}{2}, x; \frac{1}{2}, 0, \frac{1}{2}$ |
| (21) $\bar{3}^- x, x, x; 0, 0, 0$ | (22) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; 0, 0, \frac{1}{2}$ | (23) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (24) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{2}, 0, 0$ |

For ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+ set

- | | | | |
|---|---|---|--|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, \frac{1}{4}, z$ | (3) $2 \quad \frac{1}{4}, y, 0$ | (4) $2 \quad x, 0, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, x, x$ | (6) $3^+(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ | (7) $3^+(\frac{1}{6}, \frac{1}{6}, \frac{1}{6}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (8) $3^+(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, x, x$ | (10) $3^-(\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^-(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^-(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $\bar{1} \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (14) $b \quad x, y, 0$ | (15) $a \quad x, 0, z$ | (16) $c \quad 0, y, z$ |
| (17) $\bar{3}^+ x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (18) $\bar{3}^+ \bar{x} - \frac{1}{2}, x, \bar{x}; -\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (19) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; -\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+ \bar{x}, \bar{x} - \frac{1}{2}, x; \frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ |
| (21) $\bar{3}^- x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (22) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (23) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (24) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$				h,k,l cyclically permutable General:	
48 <i>e</i> 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) \bar{x},\bar{y},\bar{z} (17) \bar{z},\bar{x},\bar{y} (21) \bar{y},\bar{z},\bar{x}	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$ (10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (14) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (18) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ (22) $y, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$ (15) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (19) $z + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (23) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (16) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (20) $z, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (24) $y + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$ $0kl : k, l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$	
24 <i>d</i> 2..	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, 0, \frac{3}{4}$ $x + \frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$	$\frac{3}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{4}, x + \frac{1}{2}, 0$	$0, \frac{1}{4}, x$ $0, \frac{3}{4}, \bar{x}$	$0, \frac{3}{4}, \bar{x} + \frac{1}{2}$ $0, \frac{1}{4}, x + \frac{1}{2}$ no extra conditions
16 <i>c</i> .3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x$	no extra conditions	
8 <i>b</i> . $\bar{3}$.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : k, l = 2n$	
8 <i>a</i> . $\bar{3}$.	0,0,0	$\frac{1}{2}, 0, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : k, l = 2n$	

Special: as above, plus

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0,0,z

Along [111] $p6$
 $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $p2mg$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I2_3$ (199)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Ia1$ ($Ibca$, 73)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
IIa	[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Ia\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (206)

Minimal non-isomorphic supergroups

I	[2] $Ia\bar{3}d$ (230)
II	[4] $Pm\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (200)

*P*432

*O*¹

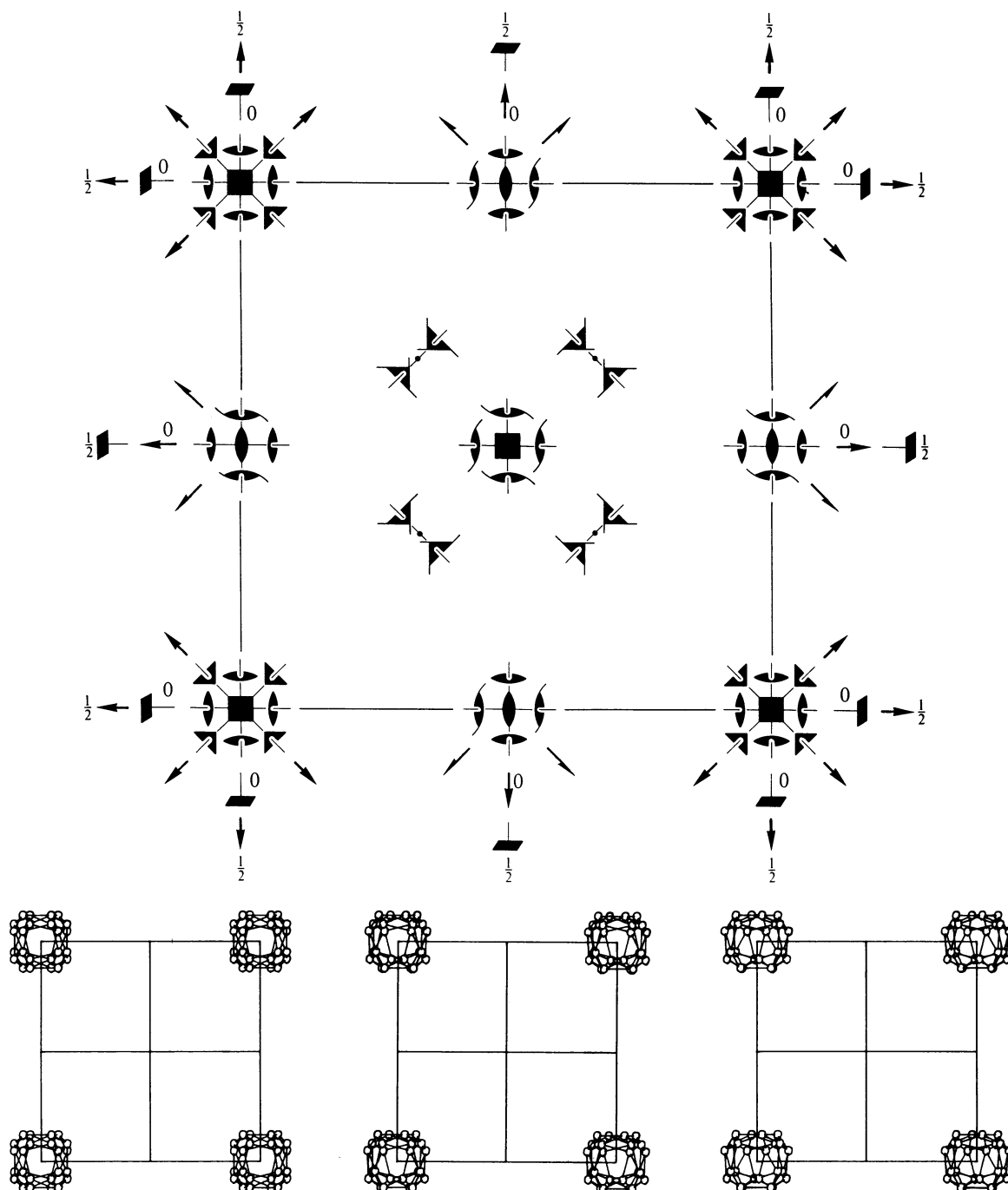
432

Cubic

No. 207

*P*432

Patterson symmetry *Pm* $\bar{3}m$



Origin at 432

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \min(x, 1-x); z \leq y$
Vertices $0,0,0 \quad 1,0,0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | | |
|-----------------------------|---|---|---|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x,\bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x,\bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) 2 $x,x,0$ | (14) 2 $x,\bar{x},0$ | (15) 4 ⁻ $0,0,z$ | (16) 4 ⁺ $0,0,z$ |
| (17) 4 ⁻ $x,0,0$ | (18) 2 $0,y,y$ | (19) 2 $0,y,\bar{y}$ | (20) 4 ⁺ $x,0,0$ |
| (21) 4 ⁺ $0,y,0$ | (22) 2 $x,0,x$ | (23) 4 ⁻ $0,y,0$ | (24) 2 $\bar{x},0,x$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

24	<i>k</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) z, x, y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}
			(9) y, z, x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x
			(13) y, x, \bar{z}	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) y, \bar{x}, z	(16) \bar{y}, x, z
			(17) x, z, \bar{y}	(18) \bar{x}, z, y	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) x, \bar{z}, y
			(21) z, y, \bar{x}	(22) z, \bar{y}, x	(23) \bar{z}, y, x	(24) $\bar{z}, \bar{y}, \bar{x}$

 h, k, l permutable

General:

no conditions

Special: no extra conditions

12	<i>j</i>	..2	$\frac{1}{2}, y, y$	$\frac{1}{2}, \bar{y}, y$	$\frac{1}{2}, y, \bar{y}$	$\frac{1}{2}, \bar{y}, \bar{y}$	$y, \frac{1}{2}, y$	$y, \frac{1}{2}, \bar{y}$
			$\bar{y}, \frac{1}{2}, y$	$\bar{y}, \frac{1}{2}, \bar{y}$	$y, y, \frac{1}{2}$	$\bar{y}, y, \frac{1}{2}$	$y, \bar{y}, \frac{1}{2}$	$\bar{y}, \bar{y}, \frac{1}{2}$
12	<i>i</i>	..2	$0, y, y$	$0, \bar{y}, y$	$0, y, \bar{y}$	$0, \bar{y}, \bar{y}$	$y, 0, y$	$y, 0, \bar{y}$
			$\bar{y}, 0, y$	$\bar{y}, 0, \bar{y}$	$y, y, 0$	$\bar{y}, y, 0$	$y, \bar{y}, 0$	$\bar{y}, \bar{y}, 0$
12	<i>h</i>	2..	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$
			$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \frac{1}{2}, x$	$0, \frac{1}{2}, \bar{x}$
8	<i>g</i>	.3.	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
			x, x, \bar{x}	$\bar{x}, \bar{x}, \bar{x}$	x, \bar{x}, x	\bar{x}, x, x		
6	<i>f</i>	4..	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
6	<i>e</i>	4..	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
3	<i>d</i>	42.2	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$			
3	<i>c</i>	42.2	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
1	<i>b</i>	432	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
1	<i>a</i>	432	$0, 0, 0$					

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [111] $p3m1$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ Origin at x, x, x Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ Origin at $x, x, 0$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \mathbf{c}$ **Maximal non-isomorphic subgroups**

I	[2] $P231$ ($P23, 195$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	{ [3] $P412$ ($P422, 89$)	1; 2; 3; 4; 13; 14; 15; 16
	{ [3] $P412$ ($P422, 89$)	1; 2; 3; 4; 17; 18; 19; 20
	{ [3] $P412$ ($P422, 89$)	1; 2; 3; 4; 21; 22; 23; 24
	{ [4] $P132$ ($R32, 155$)	1; 5; 9; 14; 19; 24
	{ [4] $P132$ ($R32, 155$)	1; 6; 12; 13; 18; 24
	{ [4] $P132$ ($R32, 155$)	1; 7; 10; 13; 19; 22
	{ [4] $P132$ ($R32, 155$)	1; 8; 11; 14; 18; 22

IIa none**IIb** [2] $F432$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (209); [4] $I432$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (211)**Maximal isomorphic subgroups of lowest index****IIc** [27] $P432$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (207)**Minimal non-isomorphic supergroups****I** [2] $Pm\bar{3}m$ (221); [2] $Pn\bar{3}n$ (222)**II** [2] $I432$ (211); [4] $F432$ (209)

$P4_232$

O^2

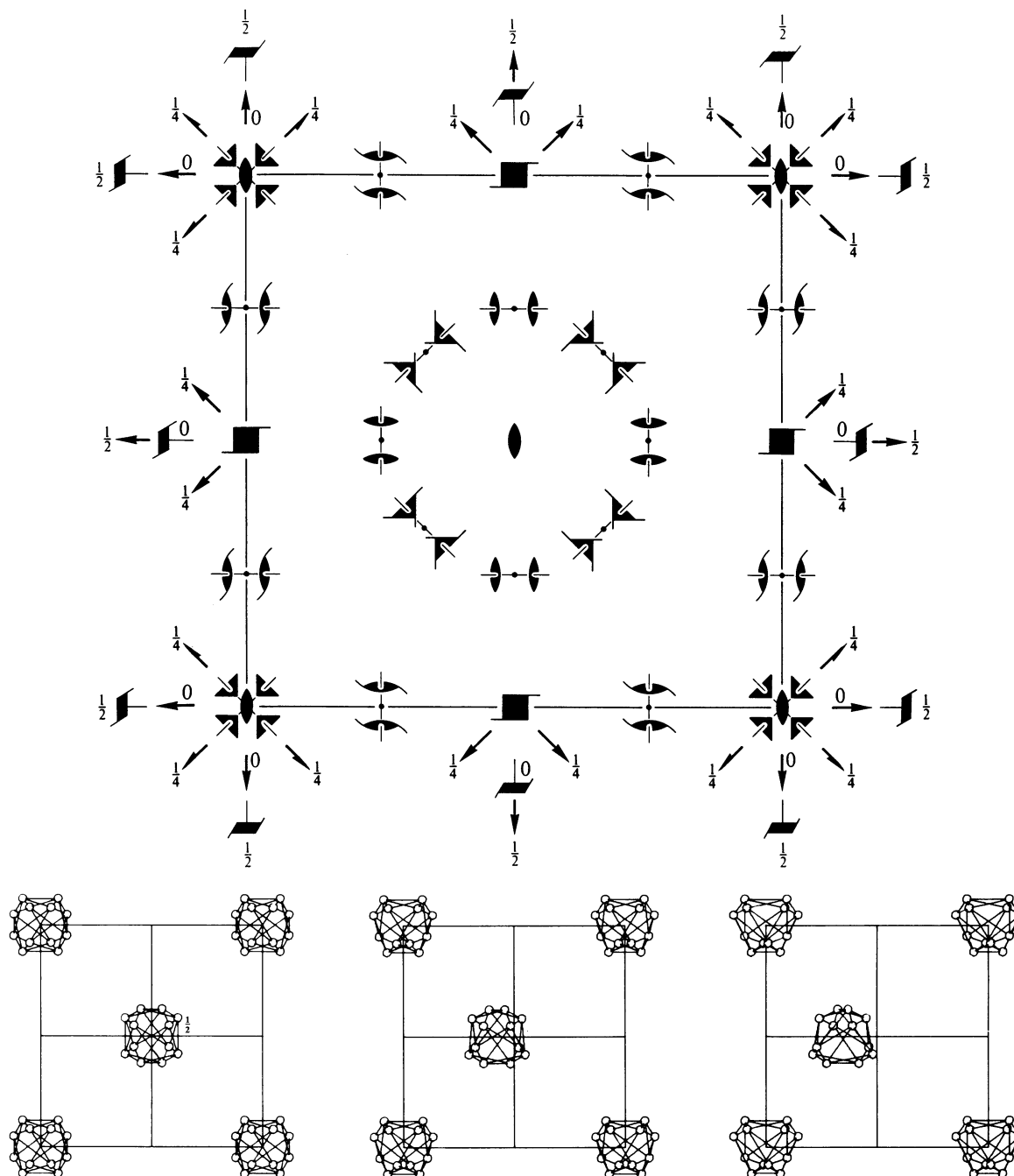
432

Cubic

No. 208

$P4_232$

Patterson symmetry $Pm\bar{3}m$



Origin at 23

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; -\frac{1}{4} \leq z \leq \frac{1}{4}; \max(-x, x - \frac{1}{2}, -y, y - \frac{1}{2}) \leq z \leq \min(x, \frac{1}{2} - x, y, \frac{1}{2} - y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

- | | | | |
|---|---|---|--|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) 2($\frac{1}{2}, \frac{1}{2}, 0$) x,x, $\frac{1}{4}$ | (14) 2 x, $\bar{x} + \frac{1}{2}, \frac{1}{4}$ | (15) 4 ⁻ (0,0, $\frac{1}{2}$) $\frac{1}{2}, 0, z$ | (16) 4 ⁺ (0,0, $\frac{1}{2}$) $0, \frac{1}{2}, z$ |
| (17) 4 ⁻ ($\frac{1}{2}, 0, 0$) x, $\frac{1}{2}, 0$ | (18) 2(0, $\frac{1}{2}, \frac{1}{2}$) $\frac{1}{4}, y, y$ | (19) 2 $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$ | (20) 4 ⁺ ($\frac{1}{2}, 0, 0$) x,0, $\frac{1}{2}$ |
| (21) 4 ⁺ (0, $\frac{1}{2}, 0$) $\frac{1}{2}, y, 0$ | (22) 2($\frac{1}{2}, 0, \frac{1}{2}$) x, $\frac{1}{4}, x$ | (23) 4 ⁻ (0, $\frac{1}{2}, 0$) 0,y, $\frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
24 <i>m</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{x}, y, \bar{z} (4) x, \bar{y}, \bar{z} (5) z, x, y (6) z, \bar{x}, \bar{y} (7) \bar{z}, \bar{x}, y (8) \bar{z}, x, \bar{y} (9) y, z, x (10) \bar{y}, z, \bar{x} (11) y, \bar{z}, \bar{x} (12) \bar{y}, \bar{z}, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	h, k, l permutable General: $h00: h = 2n$
12 <i>l</i> .. 2	$\frac{1}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$	Special: as above, plus no extra conditions
12 <i>k</i> .. 2	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$	no extra conditions
12 <i>j</i> 2..	$x, \frac{1}{2}, 0$ $0, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \frac{1}{2}, 0$ $0, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $0, x, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$ $0, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, x$ $\frac{1}{2}, 0, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x}$ $\frac{1}{2}, 0, x + \frac{1}{2}$	$hkl: h = 2n$ $hhl: l = 2n$
12 <i>i</i> 2..	$x, 0, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x}, 0, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{2}, x, 0$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, x$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $0, \frac{1}{2}, \bar{x}$ $0, \frac{1}{2}, x + \frac{1}{2}$	$hkl: h = 2n$ $hhl: l = 2n$
12 <i>h</i> 2..	$x, 0, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, 0, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $0, x, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, x$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $0, 0, \bar{x}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	$hkl: h + k + l = 2n$
8 <i>g</i> . 3.	x, x, x \bar{x}, x, \bar{x} $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ \bar{x}, \bar{x}, x x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$OkI: k + l = 2n$
6 <i>f</i> 2. 22	$\frac{1}{4}, \frac{1}{2}, 0$ $\frac{3}{4}, \frac{1}{2}, 0$ $0, \frac{1}{4}, \frac{1}{2}$ $0, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl: h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$
6 <i>e</i> 2. 22	$\frac{1}{4}, 0, \frac{1}{2}$ $\frac{3}{4}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{4}, 0$ $\frac{1}{2}, \frac{3}{4}, 0$ $0, \frac{1}{2}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	
6 <i>d</i> 222..	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$	$hkl: h + k + l = 2n$
4 <i>c</i> . 32	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl: h + k, h + l, k + l = 2n$
4 <i>b</i> . 32	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: h + k, h + l, k + l = 2n$
2 <i>a</i> 23.	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k + l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

Along [111] $p3m1$
 $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, \frac{1}{4}$

Maximal non-isomorphic subgroups

- I** [2] $P231 (P23, 195)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
 { [3] $P4_212 (P4_222, 93)$ 1; 2; 3; 4; 13; 14; 15; 16
 { [3] $P4_212 (P4_222, 93)$ 1; 2; 3; 4; 17; 18; 19; 20
 { [3] $P4_212 (P4_222, 93)$ 1; 2; 3; 4; 21; 22; 23; 24
 { [4] $P132 (R32, 155)$ 1; 5; 9; 14; 19; 24
 { [4] $P132 (R32, 155)$ 1; 6; 12; 13; 18; 24
 { [4] $P132 (R32, 155)$ 1; 7; 10; 13; 19; 22
 { [4] $P132 (R32, 155)$ 1; 8; 11; 14; 18; 22

IIa none

IIb [2] $F4_132 (a' = 2a, b' = 2b, c' = 2c) (210)$; [4] $I4_132 (a' = 2a, b' = 2b, c' = 2c) (214)$

Maximal isomorphic subgroups of lowest index

IIc [27] $P4_232 (a' = 3a, b' = 3b, c' = 3c) (208)$

Minimal non-isomorphic supergroups

I [2] $Pm\bar{3}n (223)$; [2] $Pn\bar{3}m (224)$

II [2] $I432 (211)$; [4] $F432 (209)$

*F*432

*O*³

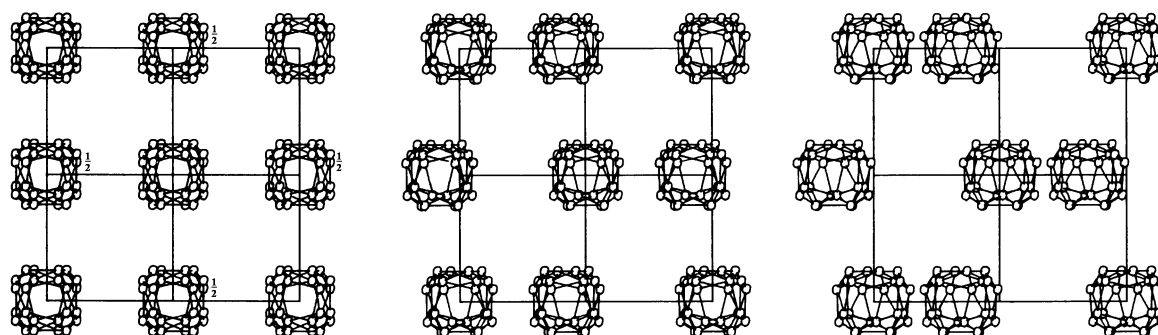
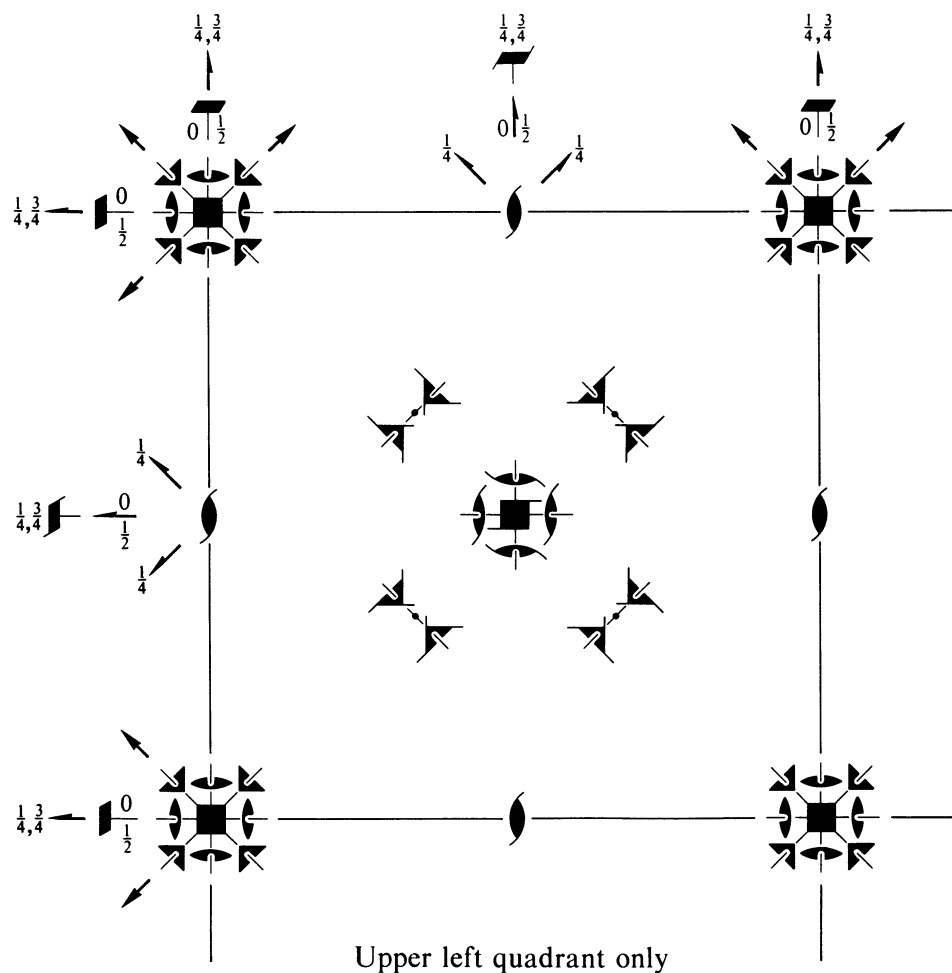
432

Cubic

No. 209

*F*432

Patterson symmetry *Fm* $\bar{3}m$



Origin at 432

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq \min(x, \frac{1}{2} - x); -y \leq z \leq y$
Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---------------------------|--|---|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) 2 x,x,0 | (14) 2 x, $\bar{x},0$ | (15) 4 ⁻ 0,0,z | (16) 4 ⁺ 0,0,z |
| (17) 4 ⁻ x,0,0 | (18) 2 0,y,y | (19) 2 0,y, \bar{y} | (20) 4 ⁺ x,0,0 |
| (21) 4 ⁺ 0,y,0 | (22) 2 x,0,x | (23) 4 ⁻ 0,y,0 | (24) 2 $\bar{x},0,x$ |

Symmetry operations (continued)For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|--|---|---|--|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2})$ $0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (4) 2 $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x - \frac{1}{3}, x - \frac{1}{3}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{3}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{4}, \frac{1}{4}, 0)$ $x, x + \frac{1}{4}, \frac{1}{4}$ | (14) $2(-\frac{1}{4}, \frac{1}{4}, 0)$ $x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ | (15) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{2})$ $-\frac{1}{4}, \frac{1}{4}, z$ |
| (17) $4^- x, \frac{1}{2}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2})$ $0, y, y$ | (19) 2 $0, y + \frac{1}{2}, \bar{y}$ | (20) $4^+ x, 0, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (22) $2(\frac{1}{4}, 0, \frac{1}{4})$ $x - \frac{1}{4}, \frac{1}{4}, x$ | (23) $4^-(0, \frac{1}{2}, 0)$ $-\frac{1}{4}, y, \frac{1}{4}$ | (24) $2(-\frac{1}{4}, 0, \frac{1}{4})$ $\bar{x} + \frac{1}{4}, \frac{1}{4}, x$ |

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- | | | | |
|--|---|--|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} + \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x - \frac{1}{6}, x - \frac{1}{6}, x$ | (10) $3^- x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) $3^-(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ |
| (13) $2(\frac{1}{4}, \frac{1}{4}, 0)$ $x, x - \frac{1}{4}, \frac{1}{4}$ | (14) $2(\frac{1}{4}, -\frac{1}{4}, 0)$ $x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ | (15) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{4}, -\frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (18) $2(0, \frac{1}{4}, \frac{1}{4})$ $\frac{1}{4}, y - \frac{1}{4}, y$ | (19) $2(0, -\frac{1}{4}, \frac{1}{4})$ $\frac{1}{4}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0)$ $x, -\frac{1}{4}, \frac{1}{4}$ |
| (21) $4^+ \frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, x$ | (23) $4^- 0, y, \frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, 0, x$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|--|---|--|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, x + \frac{1}{6}, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{6}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^- x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^-(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$ | (14) 2 $x, \bar{x} + \frac{1}{2}, 0$ | (15) $4^- \frac{1}{2}, 0, z$ | (16) $4^+ 0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, -\frac{1}{4}$ | (18) $2(0, \frac{1}{4}, \frac{1}{4})$ $\frac{1}{4}, y + \frac{1}{4}, y$ | (19) $2(0, \frac{1}{4}, -\frac{1}{4})$ $\frac{1}{4}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ |
| (21) $4^+(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, -\frac{1}{4}$ | (22) $2(\frac{1}{4}, 0, \frac{1}{4})$ $x + \frac{1}{4}, \frac{1}{4}, x$ | (23) $4^-(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (24) $2(\frac{1}{4}, 0, -\frac{1}{4})$ $\bar{x} + \frac{1}{4}, \frac{1}{4}, x$ |

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0, 0, 0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ $(\frac{1}{2}, 0, \frac{1}{2})+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

Reflection conditions

 h, k, l permutable

General:

 $hkl : h + k, h + l, k + l = 2n$ $OkI : k, l = 2n$ $hhl : h + l = 2n$ $h00 : h = 2n$

Special: as above, plus

 $hkl : h = 2n$

no extra conditions

no extra conditions

no extra conditions

no extra conditions

 $hkl : h = 2n$ $hkl : h = 2n$

no extra conditions

no extra conditions

96	j	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) z, x, y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}
			(9) y, z, x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x
			(13) y, x, \bar{z}	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) y, \bar{x}, z	(16) \bar{y}, x, z
			(17) x, z, \bar{y}	(18) \bar{x}, z, y	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) x, \bar{z}, y
			(21) z, y, \bar{x}	(22) z, \bar{y}, x	(23) \bar{z}, y, x	(24) $\bar{z}, \bar{y}, \bar{x}$

48	i	2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, x$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$
			$\frac{1}{4}, x, \frac{3}{4}$	$\frac{3}{4}, \bar{x}, \frac{3}{4}$	$x, \frac{1}{4}, \frac{3}{4}$	$\bar{x}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \bar{x}$	$\frac{1}{4}, \frac{3}{4}, x$

48	h	..2	$\frac{1}{2}, y, y$	$\frac{1}{2}, \bar{y}, y$	$\frac{1}{2}, y, \bar{y}$	$\frac{1}{2}, \bar{y}, \bar{y}$	$y, \frac{1}{2}, y$	$y, \frac{1}{2}, \bar{y}$
			$\bar{y}, \frac{1}{2}, y$	$\bar{y}, \frac{1}{2}, \bar{y}$	$y, y, \frac{1}{2}$	$\bar{y}, y, \frac{1}{2}$	$y, \bar{y}, \frac{1}{2}$	$\bar{y}, \bar{y}, \frac{1}{2}$

48	g	..2	$0, y, y$	$0, \bar{y}, y$	$0, y, \bar{y}$	$0, \bar{y}, \bar{y}$	$y, 0, y$	$y, 0, \bar{y}$
			$\bar{y}, 0, y$	$\bar{y}, 0, \bar{y}$	$y, y, 0$	$\bar{y}, y, 0$	$y, \bar{y}, 0$	$\bar{y}, \bar{y}, 0$

32	f	.3.	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}
			x, x, \bar{x}	$\bar{x}, \bar{x}, \bar{x}$	x, \bar{x}, x	\bar{x}, x, x

24	e	4..	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
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24	d	2.22	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$
----	-----	------	-------------------------------	-------------------------------	-------------------------------	-------------------------------	-------------------------------	-------------------------------

8	c	23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$
---	-----	-----	---	---

4	b	432	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	-----	-----	---

4	a	432	$0, 0, 0$
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(Continued on page 639)

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0, 0, z

Along [111] $p3m1$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** [2] $F231$ ($F23$, 196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
 { [3] $F412$ ($I422$, 97) (1; 2; 3; 4; 13; 14; 15; 16)+
 { [3] $F412$ ($I422$, 97) (1; 2; 3; 4; 17; 18; 19; 20)+
 { [3] $F412$ ($I422$, 97) (1; 2; 3; 4; 21; 22; 23; 24)+
 { [4] $F132$ ($R32$, 155) (1; 5; 9; 14; 19; 24)+
 { [4] $F132$ ($R32$, 155) (1; 6; 12; 13; 18; 24)+
 { [4] $F132$ ($R32$, 155) (1; 7; 10; 13; 19; 22)+
 { [4] $F132$ ($R32$, 155) (1; 8; 11; 14; 18; 22)+
- IIa** { [4] $P4_232$ (208) 1; 5; 9; 14; 19; 24; (4; 6; 11; 16; 18; 23) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 7; 12; 13; 17; 21) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 { [4] $P4_232$ (208) 1; 6; 12; 13; 18; 24; (4; 5; 10; 15; 19; 23) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 7; 11; 16; 17; 22) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 { [4] $P4_232$ (208) 1; 7; 10; 13; 19; 22; (4; 8; 12; 15; 18; 21) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 6; 9; 16; 20; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 { [4] $P4_232$ (208) 1; 8; 11; 14; 18; 22; (4; 7; 9; 16; 19; 21) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 6; 10; 13; 20; 23) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 { [4] $P432$ (207) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
 { [4] $P432$ (207) 1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + $(0, \frac{1}{2}, \frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$
 { [4] $P432$ (207) 1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2}, 0, \frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2}, \frac{1}{2}, 0)$
 { [4] $P432$ (207) 1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0, \frac{1}{2}, \frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2}, \frac{1}{2}, 0)$
- IIb** none

Maximal isomorphic subgroups of lowest index

IIc [27] $F432$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (209)

Minimal non-isomorphic supergroups

- I** [2] $Fm\bar{3}m$ (225); [2] $Fm\bar{3}c$ (226)
II [2] $P432$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (207)

$F4_132$

O^4

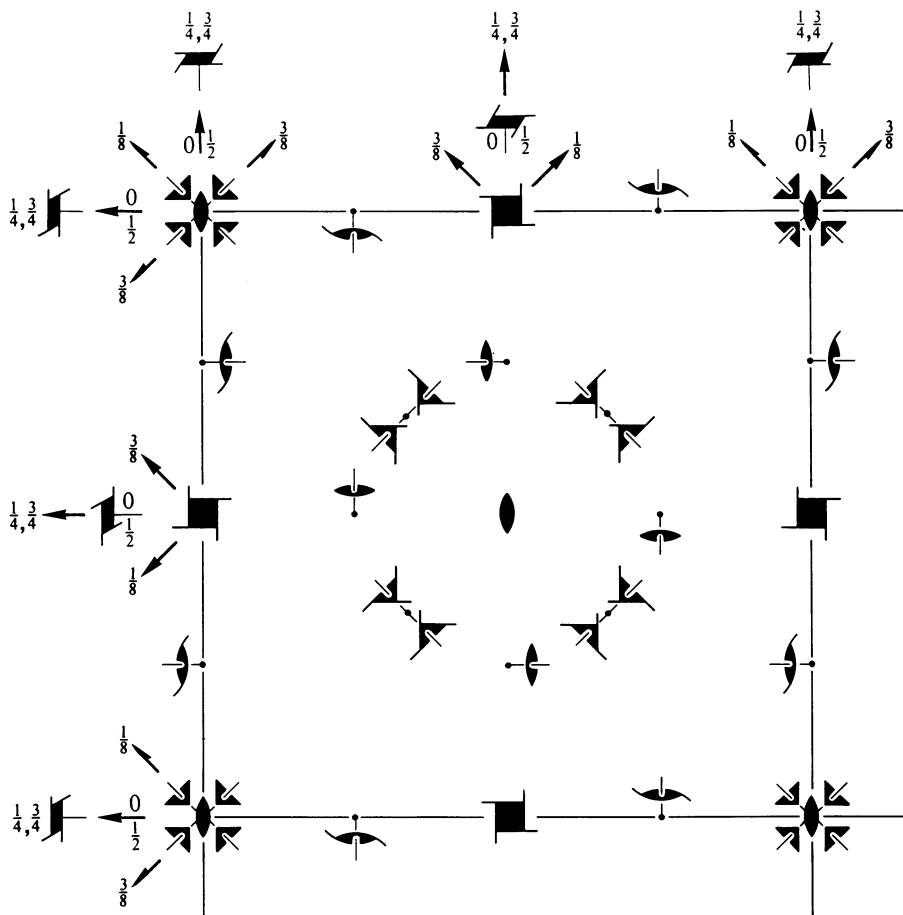
432

Cubic

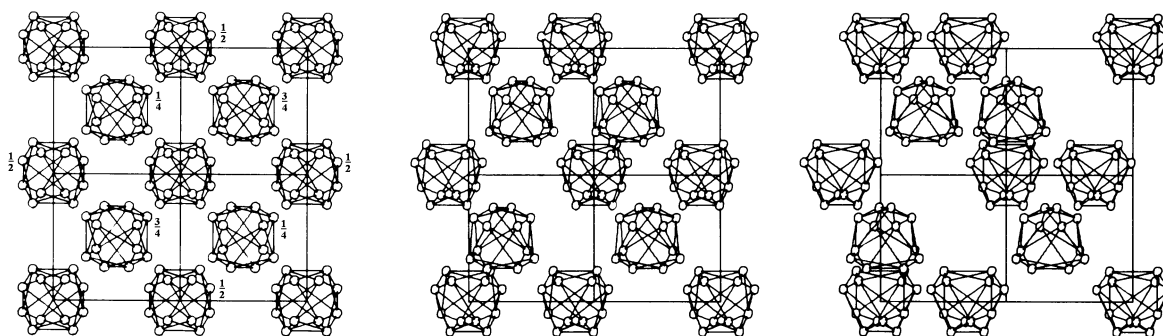
No. 210

$F4_132$

Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at 23

Asymmetric unit $0 \leq x \leq \frac{1}{2}; -\frac{1}{8} \leq y \leq \frac{1}{8}; -\frac{1}{8} \leq z \leq \frac{1}{8}; y \leq \min(x, \frac{1}{2} - x); -y \leq z \leq \min(x, \frac{1}{2} - x)$

Vertices $0, 0, 0$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ $\frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ $\frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$
 $\frac{1}{2}, 0, 0$ $\frac{3}{8}, \frac{1}{8}, \frac{1}{8}$ $\frac{3}{8}, \frac{1}{8}, -\frac{1}{8}$ $\frac{3}{8}, -\frac{1}{8}, \frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ $0, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{4}$ |
| (5) 3^+ x, x, x | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} + \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ | (7) $3^+(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{3}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{3}, x$ |
| (9) 3^- x, x, x | (10) 3^- $x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) 3^- $\bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) 3^- $\bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x - \frac{1}{4}, \frac{3}{8}$ | (14) 2 $x, \bar{x} + \frac{1}{4}, \frac{1}{8}$ | (15) $4^-(0, 0, \frac{3}{4})$ $\frac{1}{2}, \frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{4})$ $0, \frac{3}{4}, z$ |
| (17) $4^-(\frac{3}{4}, 0, 0)$ $x, \frac{1}{2}, \frac{1}{4}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2})$ $\frac{3}{8}, y + \frac{1}{4}, y$ | (19) 2 $\frac{1}{8}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{1}{4}, 0, 0)$ $x, 0, \frac{3}{4}$ |
| (21) $4^+(0, \frac{1}{4}, 0)$ $\frac{3}{4}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2})$ $x - \frac{1}{4}, \frac{3}{8}, x$ | (23) $4^-(0, \frac{3}{4}, 0)$ $\frac{1}{4}, y, \frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{4}, \frac{1}{8}, x$ |

Symmetry operations (continued)

For $(0, \frac{1}{2}, \frac{1}{2})^+$ set

- | | | | |
|---|---|---|---|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2\ 0, 0, z$ | (3) $2\ \frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0)\ x, \frac{1}{4}, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+\ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+\ x, \bar{x}, \bar{x}$ | (8) $3^+\ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^-\ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^-(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})\ \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^-\ \bar{x}, x, \bar{x}$ |
| (13) $2(\frac{3}{4}, \frac{3}{4}, 0)\ x, x, \frac{1}{8}$ | (14) $2(-\frac{1}{4}, \frac{1}{4}, 0)\ x, \bar{x} + \frac{1}{2}, \frac{3}{8}$ | (15) $4^-(0, 0, \frac{1}{4})\ \frac{1}{4}, 0, z$ | (16) $4^+(0, 0, \frac{3}{4})\ \frac{1}{4}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{3}{4}, 0, 0)\ x, \frac{1}{2}, -\frac{1}{4}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2})\ \frac{3}{8}, y - \frac{1}{4}, y$ | (19) $2\ \frac{1}{8}, y + \frac{3}{4}, \bar{y}$ | (20) $4^+(\frac{1}{4}, 0, 0)\ x, 0, \frac{1}{4}$ |
| (21) $4^+(0, \frac{3}{4}, 0)\ \frac{1}{2}, y, -\frac{1}{4}$ | (22) $2(\frac{1}{4}, 0, \frac{1}{4})\ x, \frac{1}{8}, x$ | (23) $4^-(0, \frac{1}{4}, 0)\ 0, y, \frac{3}{4}$ | (24) $2(-\frac{1}{4}, 0, \frac{1}{4})\ \bar{x} + \frac{1}{2}, \frac{3}{8}, x$ |

For $(\frac{1}{2}, 0, \frac{1}{2})^+$ set

- | | | | |
|---|--|---|---|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2\ \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0, \frac{1}{2}, 0)\ 0, y, \frac{1}{4}$ | (4) $2\ x, 0, 0$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+\ \bar{x}, x, \bar{x}$ | (7) $3^+\ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+\ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x - \frac{1}{6}, x - \frac{1}{3}, x$ | (10) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^-\ \bar{x}, \bar{x}, x$ | (12) $3^-\ \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{4}, \frac{1}{4}, 0)\ x, x, \frac{1}{8}$ | (14) $2(\frac{1}{4}, -\frac{1}{4}, 0)\ x, \bar{x} + \frac{1}{2}, \frac{3}{8}$ | (15) $4^-(0, 0, \frac{1}{4})\ \frac{3}{4}, 0, z$ | (16) $4^+(0, 0, \frac{3}{4})\ -\frac{1}{4}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0)\ x, \frac{1}{4}, 0$ | (18) $2(0, \frac{3}{4}, \frac{3}{4})\ \frac{1}{8}, y, y$ | (19) $2(0, -\frac{1}{4}, \frac{1}{4})\ \frac{3}{8}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0)\ x, \frac{1}{4}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{4}, 0)\ \frac{1}{4}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2})\ x + \frac{1}{4}, \frac{3}{8}, x$ | (23) $4^-(0, \frac{3}{4}, 0)\ -\frac{1}{4}, y, \frac{1}{2}$ | (24) $2\ \bar{x} + \frac{3}{4}, \frac{1}{8}, x$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)^+$ set

- | | | | |
|---|--|---|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2(0, 0, \frac{1}{2})\ \frac{1}{4}, 0, z$ | (3) $2\ 0, y, 0$ | (4) $2\ x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x + \frac{1}{6}, x + \frac{1}{3}, x$ | (6) $3^+\ \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+\ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+\ \bar{x}, \bar{x}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\ x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^-\ x, \bar{x}, \bar{x}$ | (11) $3^-\ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^-(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})\ \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0)\ x, x + \frac{1}{4}, \frac{3}{8}$ | (14) $2\ x, \bar{x} + \frac{3}{4}, \frac{1}{8}$ | (15) $4^-(0, 0, \frac{3}{4})\ \frac{1}{2}, -\frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{4})\ 0, \frac{1}{4}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0)\ x, \frac{3}{4}, 0$ | (18) $2(0, \frac{1}{4}, \frac{1}{4})\ \frac{1}{8}, y, y$ | (19) $2(0, \frac{1}{4}, -\frac{1}{4})\ \frac{3}{8}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0)\ x, -\frac{1}{4}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{3}{4}, 0)\ \frac{1}{2}, y, \frac{1}{4}$ | (22) $2(\frac{3}{4}, 0, \frac{3}{4})\ x, \frac{1}{8}, x$ | (23) $4^-(0, \frac{1}{4}, 0)\ 0, y, \frac{1}{4}$ | (24) $2(\frac{1}{4}, 0, -\frac{1}{4})\ \bar{x} + \frac{1}{2}, \frac{3}{8}, x$ |

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	(0, 0, 0) ⁺	(0, $\frac{1}{2}$, $\frac{1}{2}$) ⁺	($\frac{1}{2}$, 0, $\frac{1}{2}$) ⁺	($\frac{1}{2}$, $\frac{1}{2}$, 0) ⁺	Reflection conditions
					h, k, l permutable
					General:

96	$h\ 1$	(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$	$hkl : h + k = 2n$ and $h + l, k + l = 2n$
		(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$	(7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	$0kl : k, l = 2n$
		(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	(11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	(12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	$hhl : h + l = 2n$
		(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$	(14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$	(16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	$h00 : h = 4n$
		(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$	(19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$	
		(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$	(23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$	(24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	

Special: as above, plus

48	$g\ \dots 2$	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$	$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$	no extra conditions
		$\bar{y} + \frac{1}{4}, \frac{1}{8}, y$	$\bar{y} + \frac{3}{4}, \frac{7}{8}, \bar{y} + \frac{1}{2}$	$y + \frac{3}{4}, \frac{3}{8}, y + \frac{1}{2}$	$y + \frac{1}{4}, \frac{5}{8}, \bar{y}$	
		$y, \bar{y} + \frac{1}{4}, \frac{1}{8}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{7}{8}$	$y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{8}$	$\bar{y}, y + \frac{1}{4}, \frac{5}{8}$	

48	$f\ 2..$	$x, 0, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$0, 0, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$	$hkl : h = 2n + 1$
		$\frac{3}{4}, x + \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{1}{4}$	$x + \frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, x + \frac{3}{4}$	or $h + k + l = 4n$

32	$e\ .3.$	x, x, x	$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$	$0kl : k + l = 4n$
		$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$x + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	

16	$d\ .32$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{3}{8}, \frac{7}{8}$	} $hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$
16	$c\ .32$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$	

8	$b\ 23.$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	} $hkl : h = 2n + 1$ or $h + k + l = 4n$
8	$a\ 23.$	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{4}, 0, z$

Along [111] $p3m1$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, \frac{1}{8}$

Maximal non-isomorphic subgroups

- I** $[2] F 231 (F 23, 196)$ $(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+$
 $[3] F 4_1 12 (I 4_1 22, 98)$ $(1; 2; 3; 4; 13; 14; 15; 16)+$
 $[3] F 4_1 12 (I 4_1 22, 98)$ $(1; 2; 3; 4; 17; 18; 19; 20)+$
 $[3] F 4_1 12 (I 4_1 22, 98)$ $(1; 2; 3; 4; 21; 22; 23; 24)+$
 $[4] F 132 (R 32, 155)$ $(1; 5; 9; 14; 19; 24)+$
 $[4] F 132 (R 32, 155)$ $(1; 6; 12; 13; 18; 24)+$
 $[4] F 132 (R 32, 155)$ $(1; 7; 10; 13; 19; 22)+$
 $[4] F 132 (R 32, 155)$ $(1; 8; 11; 14; 18; 22)+$
- IIa** $[4] P 4_1 32 (213)$ $1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24$
 $[4] P 4_1 32 (213)$ $1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + (0, \frac{1}{2}, \frac{1}{2}); (5; 6; 7; 8; 21; 22; 23;$
 $24) + (\frac{1}{2}, 0, \frac{1}{2})$
 $[4] P 4_1 32 (213)$ $1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + (\frac{1}{2}, 0, \frac{1}{2}); (5; 6; 7; 8; 13; 14; 15;$
 $16) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P 4_1 32 (213)$ $1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + (0, \frac{1}{2}, \frac{1}{2}); (9; 10; 11; 12; 13; 14; 15;$
 $16) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P 4_3 32 (212)$ $1; 5; 9; 14; 19; 24; (4; 6; 11; 16; 18; 23) + (0, \frac{1}{2}, \frac{1}{2}); (3; 8; 10; 15; 20; 22) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 7; 12;$
 $13; 17; 21) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P 4_3 32 (212)$ $1; 6; 12; 13; 18; 24; (4; 5; 10; 15; 19; 23) + (0, \frac{1}{2}, \frac{1}{2}); (3; 7; 11; 16; 17; 22) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 8; 9;$
 $14; 20; 21) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P 4_3 32 (212)$ $1; 7; 10; 13; 19; 22; (4; 8; 12; 15; 18; 21) + (0, \frac{1}{2}, \frac{1}{2}); (3; 6; 9; 16; 20; 24) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 5; 11;$
 $14; 17; 23) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P 4_3 32 (212)$ $1; 8; 11; 14; 18; 22; (4; 7; 9; 16; 19; 21) + (0, \frac{1}{2}, \frac{1}{2}); (3; 5; 12; 15; 17; 24) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 6; 10;$
 $13; 20; 23) + (\frac{1}{2}, \frac{1}{2}, 0)$
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** $[27] F 4_1 32 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (210)$

Minimal non-isomorphic supergroups

- I** $[2] F d \bar{3} m (227); [2] F d \bar{3} c (228)$
II $[2] P 4_2 32 (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (208)$

*I*432

O^5

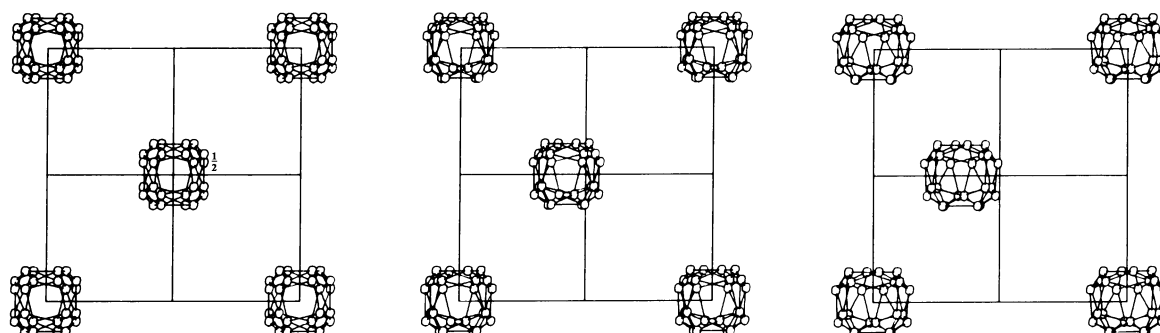
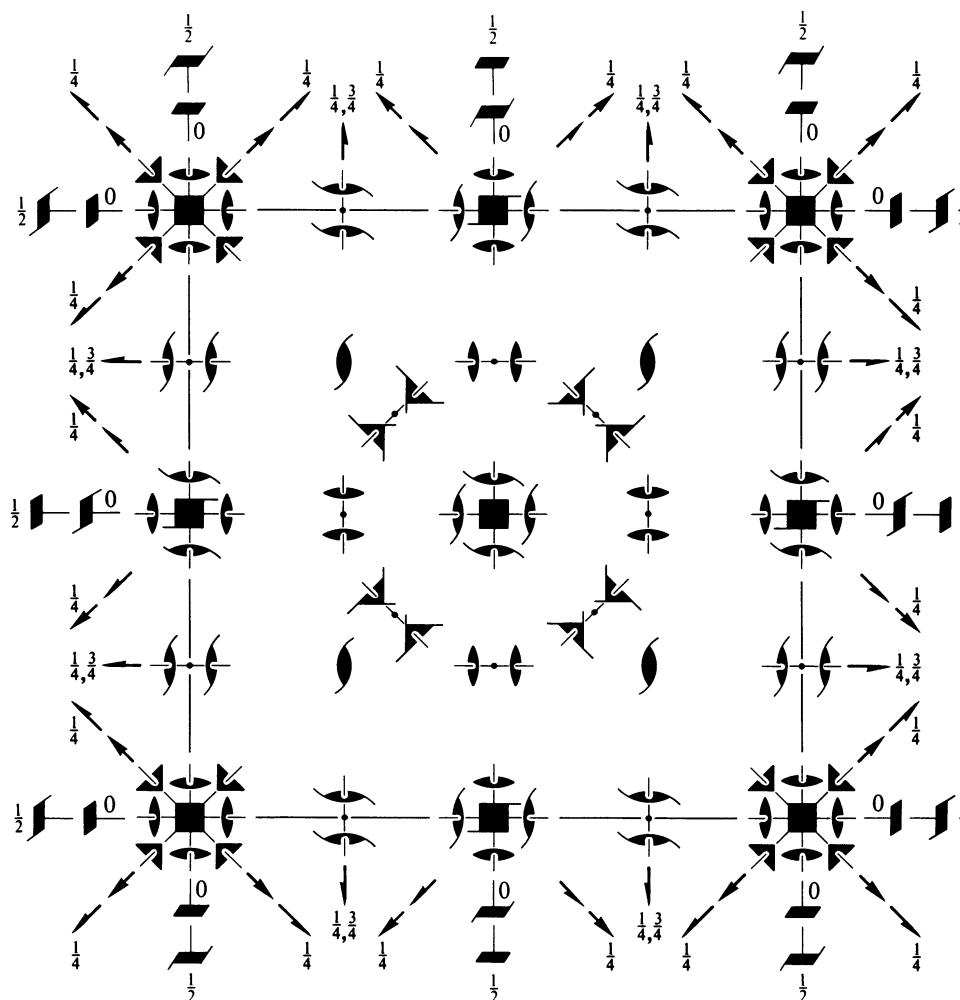
432

Cubic

No. 211

*I*432

Patterson symmetry $Im\bar{3}m$



Origin at 432

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; z \leq \min(x, \frac{1}{2} - x, y, \frac{1}{2} - y)$
 Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---------------------------|--|--|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x} ,x, \bar{x} | (7) 3 ⁺ x, \bar{x} , \bar{x} | (8) 3 ⁺ \bar{x} , \bar{x} ,x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x} , \bar{x} | (11) 3 ⁻ \bar{x} , \bar{x} ,x | (12) 3 ⁻ \bar{x} ,x, \bar{x} |
| (13) 2 x,x,0 | (14) 2 x, \bar{x} ,0 | (15) 4 ⁻ 0,0,z | (16) 4 ⁺ 0,0,z |
| (17) 4 ⁻ x,0,0 | (18) 2 0,y,y | (19) 2 0,y, \bar{y} | (20) 4 ⁺ x,0,0 |
| (21) 4 ⁺ 0,y,0 | (22) 2 x,0,x | (23) 4 ⁻ 0,y,0 | (24) 2 \bar{x} ,0,x |

For ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2($\frac{1}{2}$,0,0) $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x | (6) 3 ⁺ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$ | (7) 3 ⁺ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$ | (8) 3 ⁺ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$ |
| (9) 3 ⁻ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x | (10) 3 ⁻ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$ | (11) 3 ⁻ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$ | (12) 3 ⁻ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$ |
| (13) 2($\frac{1}{2}, \frac{1}{2}$,0) x,x, $\frac{1}{4}$ | (14) 2 x, $\bar{x} + \frac{1}{2}, \frac{1}{4}$ | (15) 4 ⁻ (0,0, $\frac{1}{2}$) $\frac{1}{2}, 0, z$ | (16) 4 ⁺ (0,0, $\frac{1}{2}$) $0, \frac{1}{2}, z$ |
| (17) 4 ⁻ ($\frac{1}{2}$,0,0) x, $\frac{1}{2}$,0 | (18) 2(0, $\frac{1}{2}, \frac{1}{2}$) $\frac{1}{4}, y, y$ | (19) 2 $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$ | (20) 4 ⁺ ($\frac{1}{2}$,0,0) x,0, $\frac{1}{2}$ |
| (21) 4 ⁺ (0, $\frac{1}{2}$,0) $\frac{1}{2}, y, 0$ | (22) 2($\frac{1}{2}$,0, $\frac{1}{2}$) x, $\frac{1}{4}, x$ | (23) 4 ⁻ (0, $\frac{1}{2}$,0) 0,y, $\frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions		
	(0,0,0)+ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+						
48 j 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) y,x, \bar{z} (17) x,z, \bar{y} (21) z,y, \bar{x}	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y}, \bar{x}, \bar{z}$ (18) \bar{x}, z, y (22) z, \bar{y}, x	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, z (19) $\bar{x}, \bar{z}, \bar{y}$ (23) \bar{z}, y, x	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, z (20) x, \bar{z}, y (24) $\bar{z}, \bar{y}, \bar{x}$	hkl : h + k + l = 2n Okl : k + l = 2n hhl : l = 2n h00 : h = 2n Special: as above, plus		
24 i .. 2	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ y, $\bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ y, $y + \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$	no extra conditions		
24 h .. 2	0,y,y $\bar{y}, 0, y$	0, \bar{y}, y $\bar{y}, 0, \bar{y}$	0,y, \bar{y} y,y,0	0, \bar{y}, \bar{y} $\bar{y}, y, 0$	y,0,y y, $\bar{y}, 0$	y,0, \bar{y} $\bar{y}, \bar{y}, 0$	no extra conditions
24 g 2..	x, $\frac{1}{2}, 0$ $\frac{1}{2}, x, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x}, 0$	0,x, $\frac{1}{2}$ x,0, $\frac{1}{2}$	0, $\bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, x$ 0, $\frac{1}{2}, \bar{x}$	$\frac{1}{2}, 0, \bar{x}$ 0, $\frac{1}{2}, x$	no extra conditions
16 f .3.	x,x,x x,x, \bar{x}	\bar{x}, \bar{x}, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x	no extra conditions		
12 e 4..	x,0,0	$\bar{x}, 0, 0$	0,x,0	0, $\bar{x}, 0$	0,0,x	0,0, \bar{x}	no extra conditions
12 d 2.22	$\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, \frac{1}{2}, 0$	0, $\frac{1}{4}, \frac{1}{2}$	0, $\frac{3}{4}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	no extra conditions
8 c .32	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	hkl : k, l = 2n		
6 b 42.2	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions			
2 a 432	0,0,0	no extra conditions					

Symmetry of special projections

Along [001] $p4mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ Origin at 0,0,z	Along [111] $p3m1$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x,x,x	Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at x,x,0
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(Continued on page 645)

Maximal non-isomorphic subgroups

- I** [2] $I231 (I23, 197)$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
 { [3] $I412 (I422, 97)$ (1; 2; 3; 4; 13; 14; 15; 16)+
 { [3] $I412 (I422, 97)$ (1; 2; 3; 4; 17; 18; 19; 20)+
 { [3] $I412 (I422, 97)$ (1; 2; 3; 4; 21; 22; 23; 24)+
 { [4] $I132 (R32, 155)$ (1; 5; 9; 14; 19; 24)+
 { [4] $I132 (R32, 155)$ (1; 6; 12; 13; 18; 24)+
 { [4] $I132 (R32, 155)$ (1; 7; 10; 13; 19; 22)+
 { [4] $I132 (R32, 155)$ (1; 8; 11; 14; 18; 22)+
- IIa** [2] $P4_232 (208)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P432 (207)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [27] $I432 (a' = 3a, b' = 3b, c' = 3c) (211)$

Minimal non-isomorphic supergroups

- I** [2] $Im\bar{3}m (229)$
- II** [4] $P432 (a' = \frac{1}{2}a, b' = \frac{1}{2}b, c' = \frac{1}{2}c) (207)$

$P4_332$

O^6

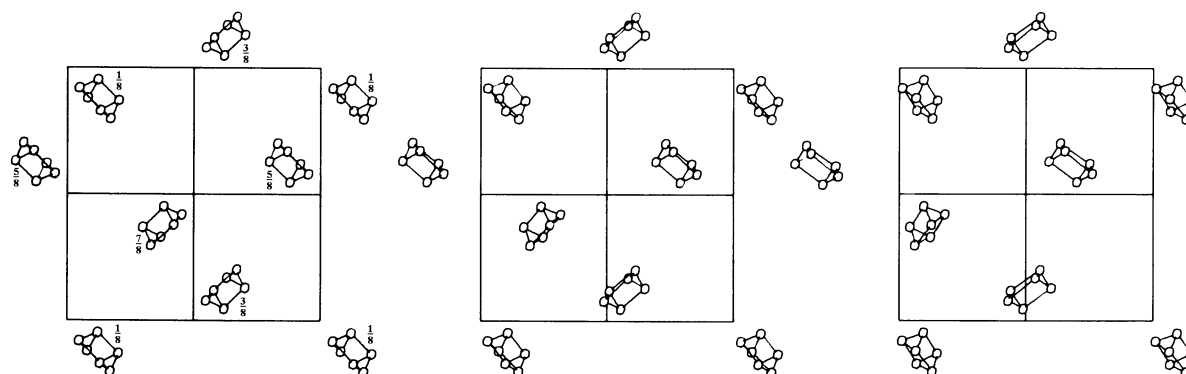
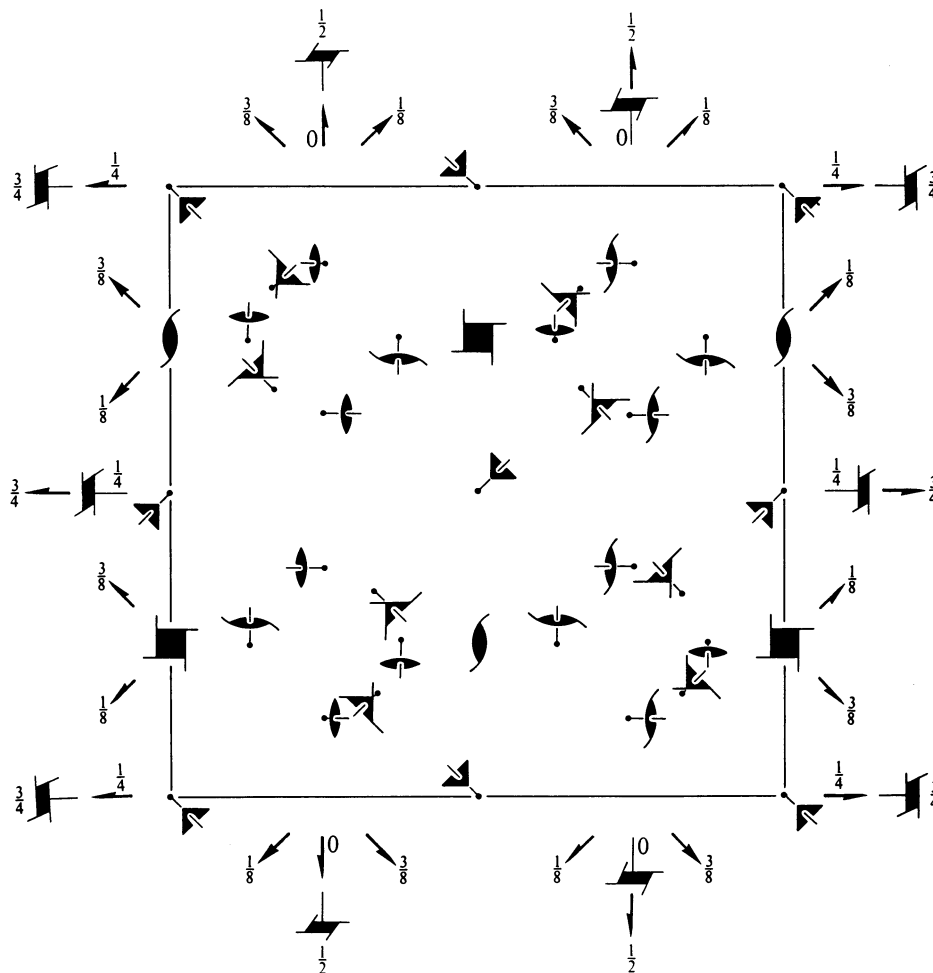
432

Cubic

No. 212

$P4_332$

Patterson symmetry $Pm\bar{3}m$



Origin on $3[111]$ at midpoint of three non-intersecting pairs of parallel screw axes 4_3 and 2_1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{3}{4}; -\frac{1}{2} \leq z \leq \frac{1}{4}; \max(-y, x - \frac{1}{2}) \leq z \leq \min(-y + \frac{1}{2}, 2x - y, 2y - x, y - 2x + \frac{1}{2})$

Vertices $0, 0, 0 \quad \frac{3}{8}, \frac{1}{8}, -\frac{1}{8} \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{3}{4}, -\frac{1}{4} \quad 0, \frac{1}{2}, -\frac{1}{2} \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \quad x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \quad \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$ | (12) $3^- (\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \quad \bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x + \frac{1}{4}, \frac{3}{8}$ | (14) $2 \quad x, \bar{x} + \frac{1}{4}, \frac{1}{8}$ | (15) $4^-(0, 0, \frac{1}{4}) \quad \frac{3}{4}, 0, z$ | (16) $4^+(0, 0, \frac{3}{4}) \quad \frac{1}{4}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{4}, 0, 0) \quad x, \frac{3}{4}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{3}{8}, y - \frac{1}{4}, y$ | (19) $2 \quad \frac{1}{8}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{3}{4}, 0, 0) \quad x, \frac{1}{4}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{3}{4}, 0) \quad \frac{1}{2}, y, \frac{1}{4}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x + \frac{1}{4}, \frac{3}{8}, x$ | (23) $4^-(0, \frac{1}{4}, 0) \quad 0, y, \frac{3}{4}$ | (24) $2 \quad \bar{x} + \frac{1}{4}, \frac{1}{8}, x$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions			
24 <i>e</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (5) z, x, y (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$ (7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (9) y, z, x (10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$ (12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (13) $y + \frac{1}{4}, x + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (15) $y + \frac{3}{4}, \bar{x} + \frac{3}{4}, z + \frac{1}{4}$ (16) $\bar{y} + \frac{3}{4}, x + \frac{1}{4}, z + \frac{3}{4}$ (17) $x + \frac{1}{4}, z + \frac{3}{4}, \bar{y} + \frac{3}{4}$ (18) $\bar{x} + \frac{3}{4}, z + \frac{1}{4}, y + \frac{3}{4}$ (19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$ (20) $x + \frac{3}{4}, \bar{z} + \frac{3}{4}, y + \frac{1}{4}$ (21) $z + \frac{1}{4}, y + \frac{3}{4}, \bar{x} + \frac{3}{4}$ (22) $z + \frac{3}{4}, \bar{y} + \frac{3}{4}, x + \frac{1}{4}$ (23) $\bar{z} + \frac{3}{4}, y + \frac{1}{4}, x + \frac{3}{4}$ (24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$h00: h = 4n$			
12 <i>d</i> .. 2	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{1}{8}, y$ $y, \bar{y} + \frac{1}{4}, \frac{1}{8}$	$\frac{3}{8}, \bar{y}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \frac{3}{8}, \bar{y}$ $\bar{y}, \bar{y} + \frac{3}{4}, \frac{3}{8}$	$\frac{7}{8}, y + \frac{1}{2}, y + \frac{1}{4}$ $y + \frac{1}{4}, \frac{7}{8}, y + \frac{1}{2}$ $y + \frac{1}{2}, y + \frac{1}{4}, \frac{7}{8}$	$\frac{5}{8}, \bar{y} + \frac{1}{2}, y + \frac{3}{4}$ $y + \frac{3}{4}, \frac{5}{8}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, y + \frac{3}{4}, \frac{5}{8}$	Special: as above, plus no extra conditions
8 <i>c</i> . 3 .	x, x, x $x + \frac{1}{4}, x + \frac{3}{4}, \bar{x} + \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{3}{4}, \bar{x} + \frac{3}{4}, x + \frac{1}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{3}{4}, x + \frac{1}{4}, x + \frac{3}{4}$	$Ok l: k = 2n + 1$ or $l = 2n + 1$ or $k + l = 4n$
4 <i>b</i> . 3 2	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{3}{8}$	$hkl: h, k = 2n + 1$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$
4 <i>a</i> . 3 2	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{5}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{7}{8}$	

Symmetry of special projections

Along [001] $p4gm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $\frac{1}{4}, \frac{1}{2}, z$	Along [111] $p3m1$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along [110] $p2gm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x + \frac{1}{4}, \frac{3}{8}$
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Maximal non-isomorphic subgroups

I	[2] $P2_131 (P2_13, 198)$	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{	[3] $P4_312 (P4_32_12, 96)$	1; 2; 3; 4; 13; 14; 15; 16
	[3] $P4_312 (P4_32_12, 96)$	1; 2; 3; 4; 17; 18; 19; 20
	[3] $P4_312 (P4_32_12, 96)$	1; 2; 3; 4; 21; 22; 23; 24
	[4] $P132 (R32, 155)$	1; 5; 9; 14; 19; 24
{	[4] $P132 (R32, 155)$	1; 6; 12; 13; 18; 24
	[4] $P132 (R32, 155)$	1; 7; 10; 13; 19; 22
	[4] $P132 (R32, 155)$	1; 8; 11; 14; 18; 22

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $P4_332 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c})$ (213); [125] $P4_332 (\mathbf{a}' = 5\mathbf{a}, \mathbf{b}' = 5\mathbf{b}, \mathbf{c}' = 5\mathbf{c})$ (212)

Minimal non-isomorphic supergroups

I none

II [2] $I4_332$ (214); [4] $F4_332$ (210)

$P4_132$

O^7

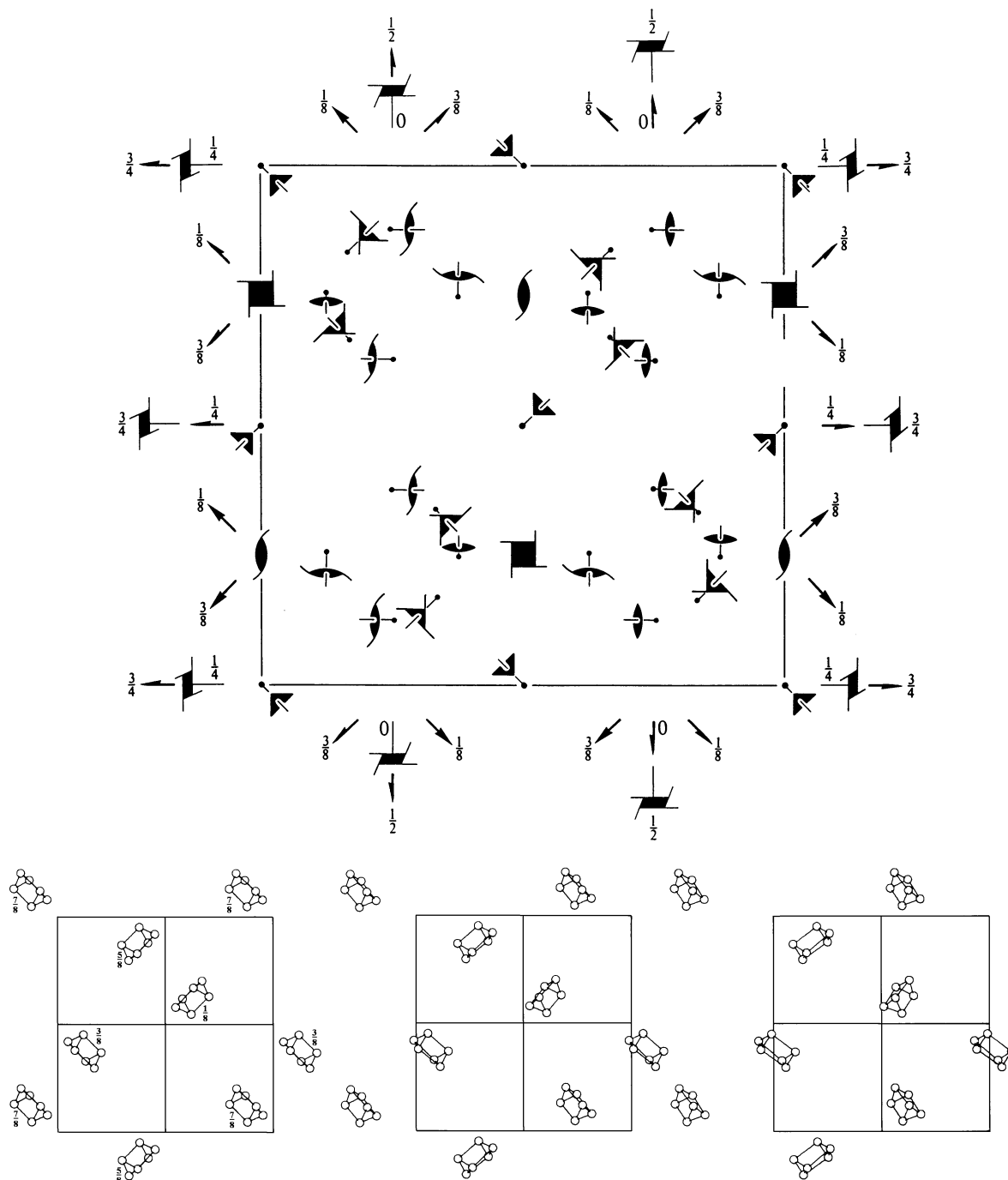
432

Cubic

No. 213

$P4_132$

Patterson symmetry $Pm\bar{3}m$



Origin on $3[111]$ at midpoint of three non-intersecting pairs of parallel screw axes 4_1 and 2_1

Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{3}{4}; 0 \leq z \leq \frac{1}{2}; x \leq y \leq x + \frac{1}{2}; (y-x)/2 \leq z \leq \min(y, (-4x-2y+3)/2, (3-2x-2y)/4)$
Vertices $0,0,0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{3}{4}, \frac{1}{4} \quad -\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad 0, \frac{1}{2}, \frac{1}{2} \quad \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},0,z$ | (3) $2(0,\frac{1}{2},0) \quad 0,y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},0$ |
| (5) $3^+ x,x,x$ | (6) $3^+ \bar{x}+\frac{1}{2},x,\bar{x}$ | (7) $3^+ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+ \bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) $3^- x,x,x$ | (10) $3^- (-\frac{1}{3},\frac{1}{3},\frac{1}{3}) \quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^- (\frac{1}{3},\frac{1}{3},-\frac{1}{3}) \quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^- (\frac{1}{3},-\frac{1}{3},\frac{1}{3}) \quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0) \quad x,x-\frac{1}{4},\frac{1}{8}$ | (14) $2 \quad x,\bar{x}+\frac{3}{4},\frac{3}{8}$ | (15) $4^-(0,0,\frac{3}{4}) \quad \frac{1}{4},0,z$ | (16) $4^+(0,0,\frac{1}{4}) \quad -\frac{1}{4},\frac{1}{2},z$ |
| (17) $4^-(\frac{3}{4},0,0) \quad x,\frac{1}{4},0$ | (18) $2(0,\frac{1}{2},\frac{1}{2}) \quad \frac{1}{8},y+\frac{1}{4},y$ | (19) $2 \quad \frac{3}{8},y+\frac{3}{4},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0) \quad x,-\frac{1}{4},\frac{1}{2}$ |
| (21) $4^+(0,\frac{1}{4},0) \quad \frac{1}{2},y,-\frac{1}{4}$ | (22) $2(\frac{1}{2},0,\frac{1}{2}) \quad x-\frac{1}{4},\frac{3}{8},x$ | (23) $4^-(0,\frac{3}{4},0) \quad 0,y,\frac{1}{4}$ | (24) $2 \quad \bar{x}+\frac{3}{4},\frac{3}{8},x$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions			
24 <i>e</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (5) z, x, y (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$ (7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (9) y, z, x (10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$ (12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (14) $\bar{y} + \frac{3}{4}, \bar{x} + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (15) $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ (16) $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ (17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{1}{4}$ (18) $\bar{x} + \frac{1}{4}, z + \frac{3}{4}, y + \frac{1}{4}$ (19) $\bar{x} + \frac{3}{4}, \bar{z} + \frac{3}{4}, \bar{y} + \frac{3}{4}$ (20) $x + \frac{1}{4}, \bar{z} + \frac{1}{4}, y + \frac{3}{4}$ (21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{1}{4}$ (22) $z + \frac{1}{4}, \bar{y} + \frac{1}{4}, x + \frac{3}{4}$ (23) $\bar{z} + \frac{1}{4}, y + \frac{3}{4}, x + \frac{1}{4}$ (24) $\bar{z} + \frac{3}{4}, \bar{y} + \frac{3}{4}, \bar{x} + \frac{3}{4}$	$h00: h = 4n$			
12 <i>d</i> .. 2	$\frac{1}{8}, y, y + \frac{1}{4}$ $y + \frac{1}{4}, \frac{1}{8}, y$ $y, y + \frac{1}{4}, \frac{1}{8}$	$\frac{3}{8}, \bar{y}, y + \frac{3}{4}$ $y + \frac{3}{4}, \frac{3}{8}, \bar{y}$ $\bar{y}, y + \frac{3}{4}, \frac{3}{8}$	$\frac{7}{8}, y + \frac{1}{2}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{7}{8}, y + \frac{1}{2}$ $y + \frac{1}{2}, \bar{y} + \frac{1}{4}, \frac{7}{8}$	$\frac{5}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \frac{5}{8}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{5}{8}$	Special: as above, plus no extra conditions
8 <i>c</i> . 3 .	x, x, x $x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $\bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{4}, \bar{x} + \frac{1}{4}, x + \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	$Ok l: k = 2n + 1$ or $l = 2n + 1$ or $k + l = 4n$
4 <i>b</i> . 3 2	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{1}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{1}{8}$	$hkl: h, k = 2n + 1$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$
4 <i>a</i> . 3 2	$\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{5}{8}$	

Symmetry of special projections

Along [001] $p4gm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $\frac{1}{4}, 0, z$	Along [111] $p3m1$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along [110] $p2gm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x + \frac{1}{4}, \frac{1}{8}$
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Maximal non-isomorphic subgroups

I	[2] $P2_131 (P2_1, 3, 198)$	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{	[3] $P4_112 (P4_1, 2, 2, 92)$	1; 2; 3; 4; 13; 14; 15; 16
	[3] $P4_112 (P4_1, 2, 2, 92)$	1; 2; 3; 4; 17; 18; 19; 20
	[3] $P4_112 (P4_1, 2, 2, 92)$	1; 2; 3; 4; 21; 22; 23; 24
	[4] $P132 (R32, 155)$	1; 5; 9; 14; 19; 24
{	[4] $P132 (R32, 155)$	1; 6; 12; 13; 18; 24
	[4] $P132 (R32, 155)$	1; 7; 10; 13; 19; 22
	[4] $P132 (R32, 155)$	1; 8; 11; 14; 18; 22

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $P4_332 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (212)$; [125] $P4_132 (\mathbf{a}' = 5\mathbf{a}, \mathbf{b}' = 5\mathbf{b}, \mathbf{c}' = 5\mathbf{c}) (213)$

Minimal non-isomorphic supergroups

I none

II [2] $I4_132 (214)$; [4] $F4_132 (210)$

$I4_132$

O^8

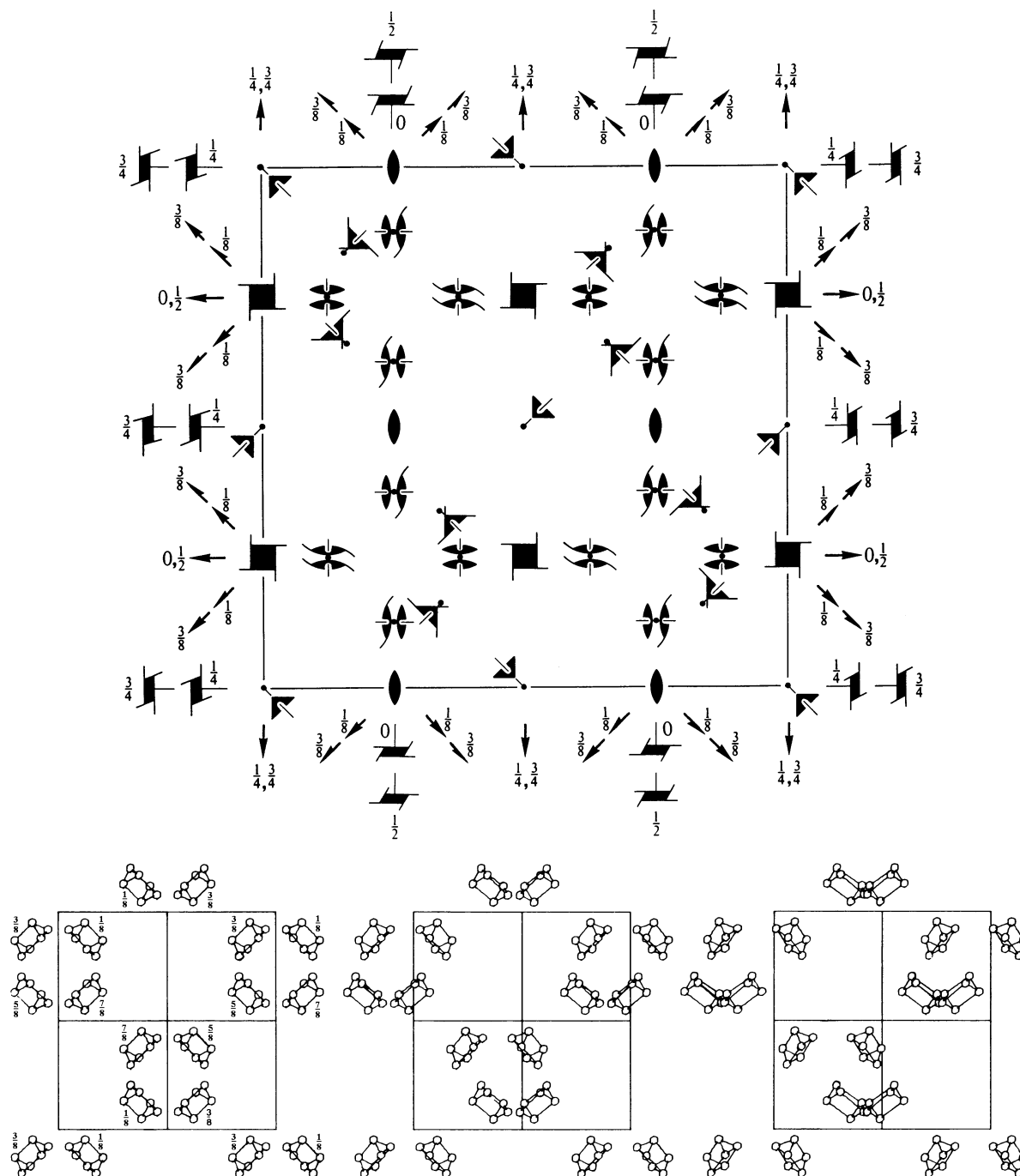
432

Cubic

No. 214

$I4_132$

Patterson symmetry $Im\bar{3}m$



Origin on $3[111]$ at midpoint of three non-intersecting pairs of parallel screw axes 4_1 and 4_3 and of three non-intersecting pairs of parallel 2 axes

Asymmetric unit $-\frac{3}{8} \leq x \leq \frac{1}{8}; -\frac{1}{8} \leq y \leq \frac{1}{8}; -\frac{1}{8} \leq z \leq \frac{3}{8}; \max(x, y, y-x-\frac{1}{8}) \leq z \leq y+\frac{1}{4}$

Vertices $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{3}{8}; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}; -\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}; -\frac{3}{8}, \frac{1}{8}, \frac{3}{8}; -\frac{3}{8}, -\frac{1}{8}, \frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--|--|--|--|
| (1) 1 | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4},0,z$ | (3) 2(0, $\frac{1}{2},0$) $0,y,\frac{1}{4}$ | (4) 2($\frac{1}{2},0,0$) $x,\frac{1}{4},0$ |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ $\bar{x}+\frac{1}{2},x,\bar{x}$ | (7) 3 ⁺ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) 3 ⁺ $\bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ ($-\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) 3 ⁻ ($\frac{1}{3},\frac{1}{3},-\frac{1}{3}$) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) 3 ⁻ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) 2($\frac{1}{2},\frac{1}{2},0$) $x,x-\frac{1}{4},\frac{1}{8}$ | (14) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$ | (15) 4 ⁻ (0,0, $\frac{3}{4}$) $\frac{1}{4},0,z$ | (16) 4 ⁺ (0,0, $\frac{1}{4}$) $-\frac{1}{4},\frac{1}{2},z$ |
| (17) 4 ⁻ ($\frac{3}{4},0,0$) $x,\frac{1}{4},0$ | (18) 2(0, $\frac{1}{2},\frac{1}{2}$) $\frac{1}{8},y+\frac{1}{4},y$ | (19) 2 $\frac{3}{8},y+\frac{3}{4},\bar{y}$ | (20) 4 ⁺ ($\frac{1}{4},0,0$) $x,-\frac{1}{4},\frac{1}{2}$ |
| (21) 4 ⁺ (0, $\frac{1}{4},0$) $\frac{1}{2},y,-\frac{1}{4}$ | (22) 2($\frac{1}{2},0,\frac{1}{2}$) $x-\frac{1}{4},\frac{1}{8},x$ | (23) 4 ⁻ (0, $\frac{3}{4},0$) $0,y,\frac{1}{4}$ | (24) 2 $\bar{x}+\frac{3}{4},\frac{3}{8},x$ |

For ($\frac{1}{2},\frac{1}{2},\frac{1}{2}$)+ set

- | | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) 2 $0,\frac{1}{4},z$ | (3) 2 $\frac{1}{4},y,0$ | (4) 2 $x,0,\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) x,x,x | (6) 3 ⁺ ($\frac{1}{6},-\frac{1}{6},\frac{1}{6}$) $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ | (7) 3 ⁺ ($-\frac{1}{6},\frac{1}{6},\frac{1}{6}$) $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (8) 3 ⁺ ($\frac{1}{6},\frac{1}{6},-\frac{1}{6}$) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ |
| (9) 3 ⁻ ($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) x,x,x | (10) 3 ⁻ ($\frac{1}{6},-\frac{1}{6},-\frac{1}{6}$) $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) 3 ⁻ ($-\frac{1}{6},-\frac{1}{6},\frac{1}{6}$) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) 3 ⁻ ($-\frac{1}{6},\frac{1}{6},-\frac{1}{6}$) $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) 2($\frac{1}{2},\frac{1}{2},0$) $x,x+\frac{1}{4},\frac{3}{8}$ | (14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$ | (15) 4 ⁻ (0,0, $\frac{1}{4}$) $\frac{3}{4},0,z$ | (16) 4 ⁺ (0,0, $\frac{3}{4}$) $\frac{1}{4},\frac{1}{2},z$ |
| (17) 4 ⁻ ($\frac{1}{4},0,0$) $x,\frac{3}{4},0$ | (18) 2(0, $\frac{1}{2},\frac{1}{2}$) $\frac{3}{8},y-\frac{1}{4},y$ | (19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$ | (20) 4 ⁺ ($\frac{3}{4},0,0$) $x,\frac{1}{4},\frac{1}{2}$ |
| (21) 4 ⁺ (0, $\frac{3}{4},0$) $\frac{1}{2},y,\frac{1}{4}$ | (22) 2($\frac{1}{2},0,\frac{1}{2}$) $x+\frac{1}{4},\frac{3}{8},x$ | (23) 4 ⁻ (0, $\frac{1}{4},0$) $0,y,\frac{3}{4}$ | (24) 2 $\bar{x}+\frac{1}{4},\frac{3}{8},x$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	(0,0,0)+ ($\frac{1}{2},\frac{1}{2},\frac{1}{2}$)+	h,k,l permutable General:
48 <i>i</i> 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y+\frac{3}{4},x+\frac{1}{4},z+\frac{1}{4}$ (17) $x+\frac{3}{4},z+\frac{1}{4},y+\frac{1}{4}$ (21) $z+\frac{3}{4},y+\frac{1}{4},x+\frac{1}{4}$ (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$ (10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$ (14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$ (18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$ (22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$ (3) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$ (7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$ (11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$ (15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$ (19) $\bar{x}+\frac{1}{4},z+\frac{3}{4},\bar{y}+\frac{3}{4}$ (23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (12) $\bar{y}+\frac{1}{2},z,x+\frac{1}{2}$ (16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$ (20) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{3}{4}$ (24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$hkl : h+k+l=2n$ $OkI : k+l=2n$ $hhl : l=2n$ $h00 : h=4n$
24 <i>h</i> ..2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$ $\bar{y}+\frac{1}{4},\frac{1}{8},y$ $y,\bar{y}+\frac{1}{4},\frac{1}{8}$ $\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$ $\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$ $\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$ $\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$ $y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$ $y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$ $\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$ $y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$	no extra conditions
24 <i>g</i> ..2	$\frac{1}{8},y,y+\frac{1}{4}$ $y+\frac{1}{4},\frac{1}{8},y$ $y,y+\frac{1}{4},\frac{1}{8}$ $\frac{3}{8},\bar{y},y+\frac{3}{4}$ $y+\frac{3}{4},\frac{3}{8},\bar{y}$ $\bar{y},y+\frac{3}{4},\frac{3}{8}$ $\frac{7}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$ $\bar{y}+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$ $y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{7}{8}$ $\frac{5}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$ $\bar{y}+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{5}{8}$	no extra conditions
24 <i>f</i> 2..	$x,0,\frac{1}{4}$ $\frac{3}{4},x+\frac{1}{4},0$ $\bar{x}+\frac{1}{2},0,\frac{3}{4}$ $\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$ $\frac{1}{4},x,0$ $x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},\bar{x}+\frac{1}{2},0$ $\bar{x}+\frac{1}{4},0,\frac{1}{4}$ $0,\frac{1}{4},x$ $0,\frac{1}{4},\bar{x}+\frac{1}{4}$ $0,\frac{3}{4},\bar{x}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$	$hkl : h=2n+1$ or $h=4n$ $hhl : h=2n+1$ or $h+k+l=4n$
16 <i>e</i> .3.	x,x,x $x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$ $\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$ $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$ $\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$ $\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	$OkI : k=2n+1$ or $k+l=4n$
12 <i>d</i> 2.22	$\frac{5}{8},0,\frac{1}{4}$ $\frac{7}{8},0,\frac{3}{4}$ $\frac{1}{4},\frac{5}{8},0$ $\frac{3}{4},\frac{7}{8},0$ $0,\frac{1}{4},\frac{5}{8}$ $0,\frac{3}{4},\frac{7}{8}$	$hkl : h,k=2n, h+k+l=4n$ or $h,k=2n+1, l=4n+2$ or $h=8n, k=8n+4$ and $h+k+l=4n+2$ or $h,k=8n+1, l=4n$ or $h=8n+1$ and $k=8n-1, l=4n$ or $h,k=8n+3, l=4n$ or $h=8n+3$ and $k=8n-3, l=4n$
12 <i>c</i> 2.22	$\frac{1}{8},0,\frac{1}{4}$ $\frac{3}{8},0,\frac{3}{4}$ $\frac{1}{4},\frac{1}{8},0$ $\frac{3}{4},\frac{3}{8},0$ $0,\frac{1}{4},\frac{1}{8}$ $0,\frac{3}{4},\frac{3}{8}$	
8 <i>b</i> .32	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$ $\frac{5}{8},\frac{1}{8},\frac{3}{8}$ $\frac{1}{8},\frac{3}{8},\frac{5}{8}$ $\frac{3}{8},\frac{5}{8},\frac{1}{8}$	$hkl : h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
8 <i>a</i> .32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{3}{8},\frac{7}{8},\frac{5}{8}$ $\frac{7}{8},\frac{5}{8},\frac{3}{8}$ $\frac{5}{8},\frac{3}{8},\frac{7}{8}$	

Symmetry of special projections

Along $[001] p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{2}, 0, z$

Along $[111] p3m1$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110] p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x + \frac{1}{4}, \frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $I2_131 (I2_13, 199)$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+

{ [3] $I4_112 (I4_122, 98)$ (1; 2; 3; 4; 13; 14; 15; 16)+

{ [3] $I4_112 (I4_122, 98)$ (1; 2; 3; 4; 17; 18; 19; 20)+

{ [3] $I4_112 (I4_122, 98)$ (1; 2; 3; 4; 21; 22; 23; 24)+

{ [4] $I132 (R32, 155)$ (1; 5; 9; 14; 19; 24)+

{ [4] $I132 (R32, 155)$ (1; 6; 12; 13; 18; 24)+

{ [4] $I132 (R32, 155)$ (1; 7; 10; 13; 19; 22)+

{ [4] $I132 (R32, 155)$ (1; 8; 11; 14; 18; 22)+

IIa [2] $P4_132 (213)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24

[2] $P4_332 (212)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $I4_132 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (214)$

Minimal non-isomorphic supergroups

I [2] $Ia\bar{3}d (230)$

II [4] $P4_232 (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (208)$

$P\bar{4}3m$

T_d^1

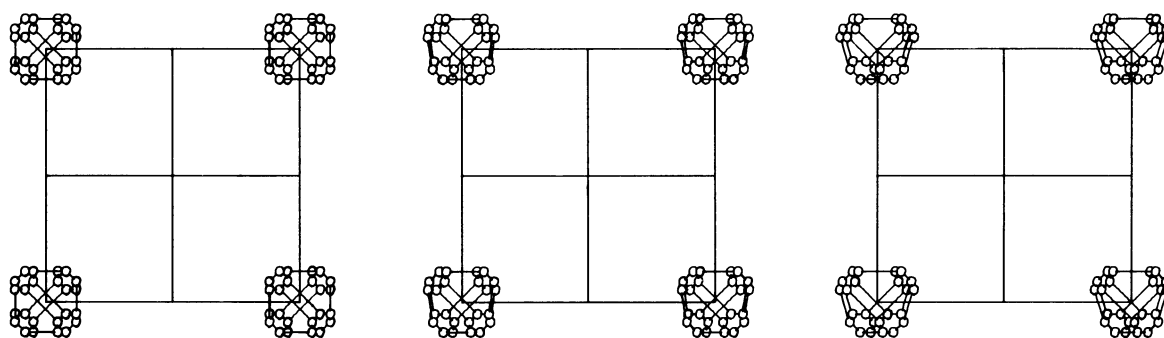
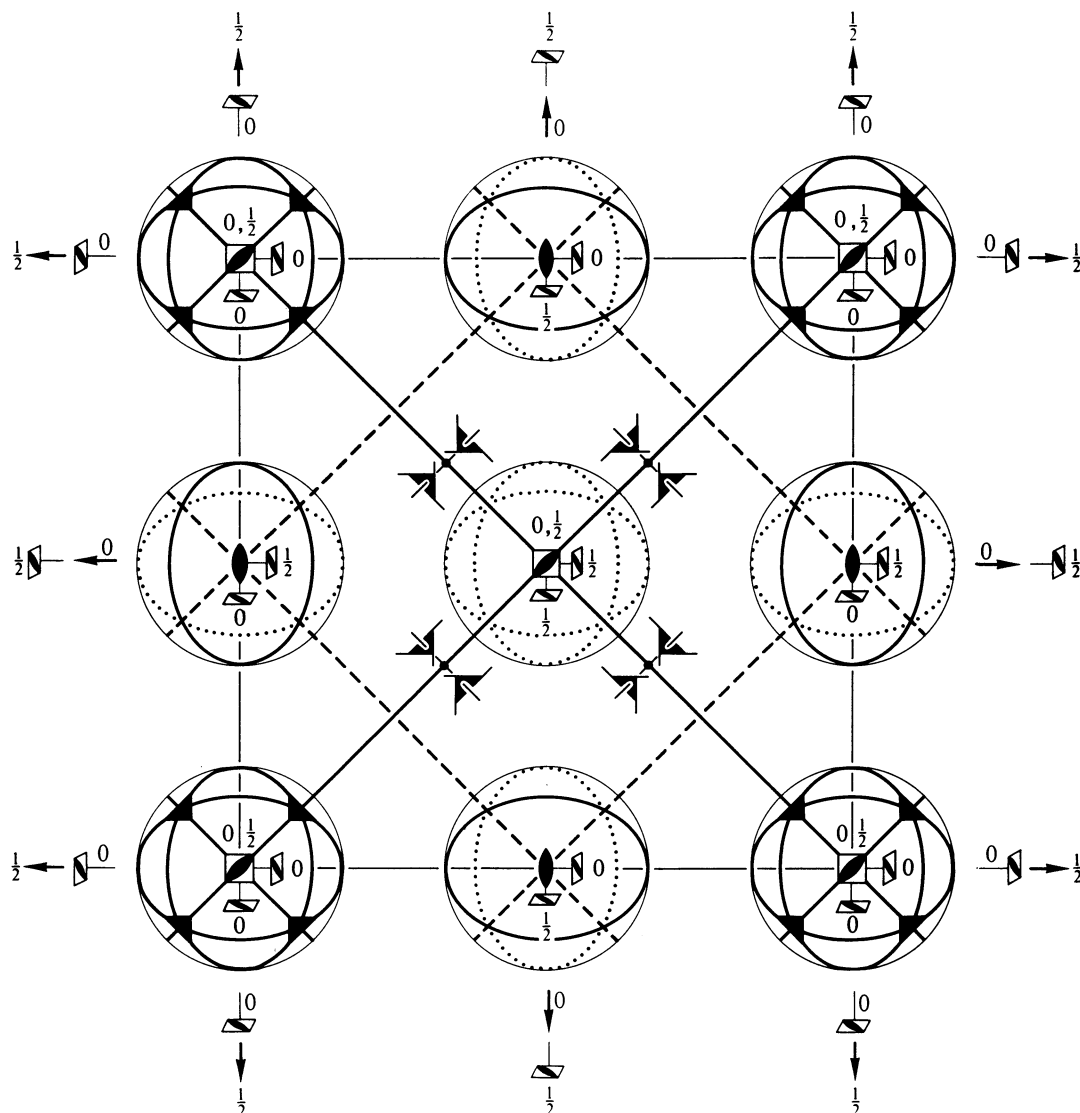
$\bar{4}3m$

Cubic

No. 215

$P\bar{4}3m$

Patterson symmetry $Pm\bar{3}m$



Origin at $\bar{4}3m$

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{2}$; $y \leq \min(x, 1-x)$; $z \leq y$

Vertices $0,0,0$ $1,0,0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | | |
|-------------------|------------------------------------|------------------------------------|------------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 2 $0,y,0$ | (4) 2 $x,0,0$ |
| (5) 3^+ x,x,x | (6) 3^+ \bar{x},x,\bar{x} | (7) 3^+ x,\bar{x},\bar{x} | (8) 3^+ \bar{x},\bar{x},x |
| (9) 3^- x,x,x | (10) 3^- x,\bar{x},\bar{x} | (11) 3^- \bar{x},\bar{x},x | (12) 3^- \bar{x},x,\bar{x} |
| (13) m x,x,z | (14) m x,\bar{x},z | (15) $\bar{4}^+$ $0,0,z$; $0,0,0$ | (16) $\bar{4}^-$ $0,0,z$; $0,0,0$ |
| (17) m x,y,y | (18) $\bar{4}^+$ $x,0,0$; $0,0,0$ | (19) $\bar{4}^-$ $x,0,0$; $0,0,0$ | (20) m x,y,\bar{y} |
| (21) m x,y,x | (22) $\bar{4}^-$ $0,y,0$; $0,0,0$ | (23) m \bar{x},y,x | (24) $\bar{4}^+$ $0,y,0$; $0,0,0$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

24	j	1	(1) x, y, z (5) z, x, y (9) y, z, x (13) y, x, z (17) x, z, y (21) z, y, x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) \bar{y}, \bar{x}, z (18) \bar{x}, z, \bar{y} (22) z, \bar{y}, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, \bar{z} (19) \bar{x}, \bar{z}, y (23) \bar{z}, y, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, \bar{z} (20) x, \bar{z}, \bar{y} (24) \bar{z}, \bar{y}, x
----	-----	---	---	--	--	--

 h, k, l permutable

General:

no conditions

Special: no extra conditions

12	i	$\dots m$	x, x, z \bar{z}, \bar{x}, x	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x}	\bar{x}, x, \bar{z} x, z, x	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x}	z, x, x x, \bar{z}, \bar{x}	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x
12	h	$2 \dots$	$x, \frac{1}{2}, 0$ $\frac{1}{2}, x, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x}, 0$	$0, x, \frac{1}{2}$ $x, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, x$ $0, \frac{1}{2}, x$	$\frac{1}{2}, 0, \bar{x}$ $0, \frac{1}{2}, \bar{x}$
6	g	$2 \dots mm$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
6	f	$2 \dots mm$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
4	e	$\dots 3m$	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
3	d	$\bar{4}2 \dots m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$			
3	c	$\bar{4}2 \dots m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
1	b	$\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
1	a	$\bar{4}3m$	$0, 0, 0$					

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0, z

Along [111] $p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ Origin at x, x, x $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Along [110] $p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ Origin at $x, x, 0$ $\mathbf{b}' = \mathbf{c}$ **Maximal non-isomorphic subgroups**

I	[2] $P231$ ($P23, 195$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{	[3] $P\bar{4}1m$ ($P\bar{4}2m, 111$)	1; 2; 3; 4; 13; 14; 15; 16
	[3] $P\bar{4}1m$ ($P\bar{4}2m, 111$)	1; 2; 3; 4; 17; 18; 19; 20
	[3] $P\bar{4}1m$ ($P\bar{4}2m, 111$)	1; 2; 3; 4; 21; 22; 23; 24
	[4] $P13m$ ($R3m, 160$)	1; 5; 9; 13; 17; 21
{	[4] $P13m$ ($R3m, 160$)	1; 6; 12; 14; 20; 21
	[4] $P13m$ ($R3m, 160$)	1; 7; 10; 14; 17; 23
	[4] $P13m$ ($R3m, 160$)	1; 8; 11; 13; 20; 23

IIa none**IIb** [2] $F\bar{4}3c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (219); [2] $F\bar{4}3m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (216); [4] $I\bar{4}3m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (217)**Maximal isomorphic subgroups of lowest index****IIc** [27] $P\bar{4}3m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (215)**Minimal non-isomorphic supergroups****I** [2] $Pm\bar{3}m$ (221); [2] $Pn\bar{3}m$ (224)**II** [2] $I\bar{4}3m$ (217); [4] $F\bar{4}3m$ (216)

$F\bar{4}3m$

T_d^2

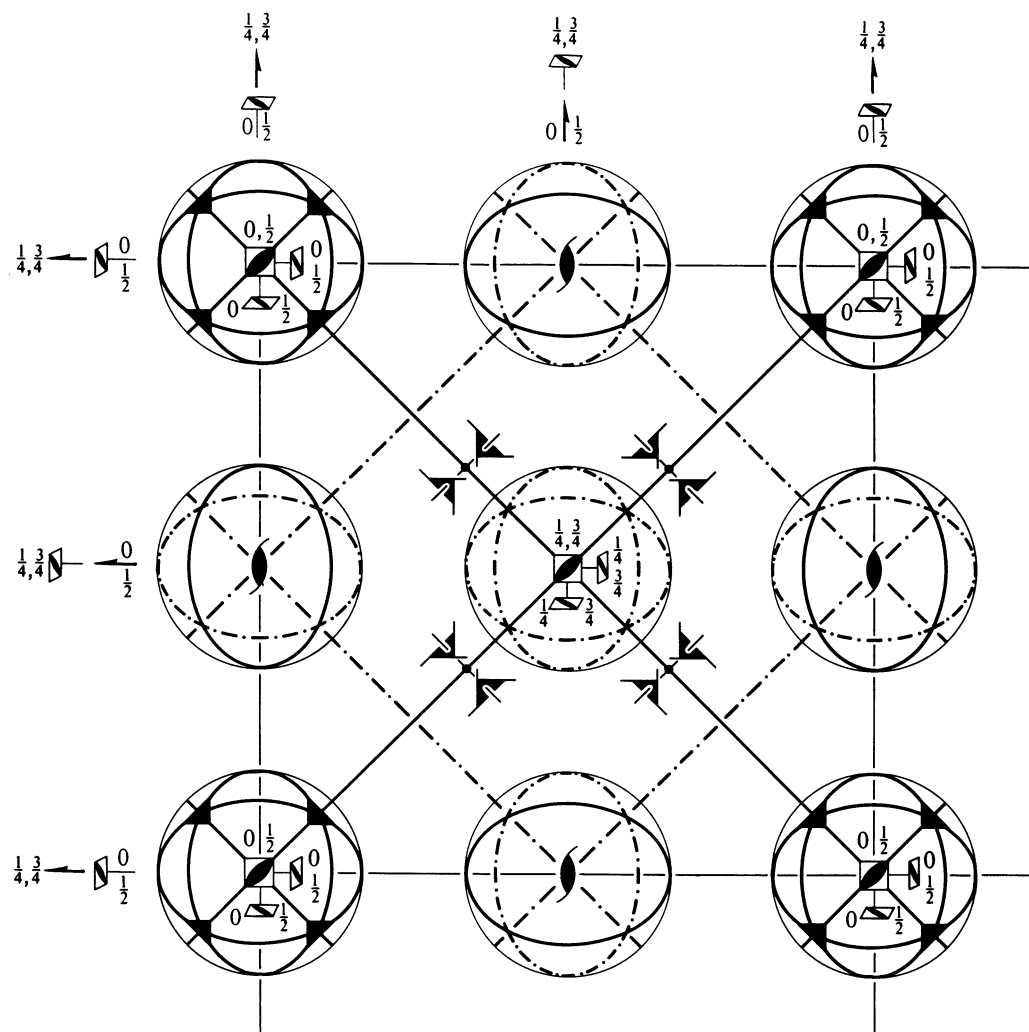
$\bar{4}3m$

Cubic

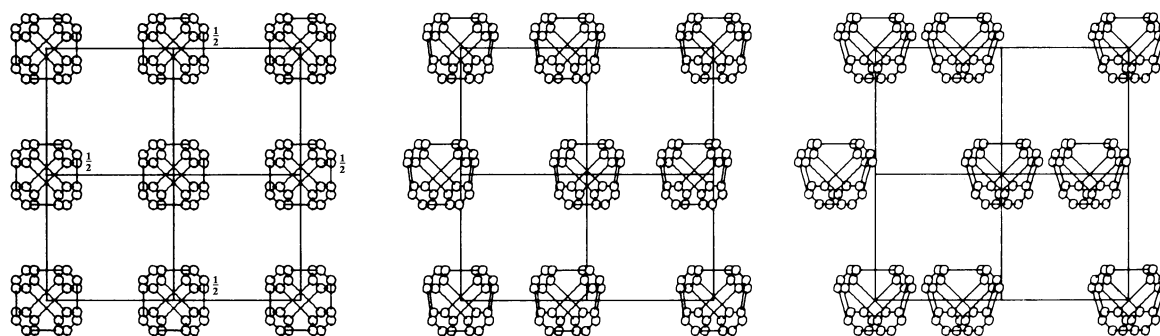
No. 216

$F\bar{4}3m$

Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at $\bar{4}3m$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $-\frac{1}{4} \leq z \leq \frac{1}{4}$; $y \leq \min(x, \frac{1}{2} - x)$; $-y \leq z \leq y$
 Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--------------------------|--|--|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x} ,x, \bar{x} | (7) 3 ⁺ x, \bar{x} , \bar{x} | (8) 3 ⁺ \bar{x} , \bar{x} ,x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x} , \bar{x} | (11) 3 ⁻ \bar{x} , \bar{x} ,x | (12) 3 ⁻ \bar{x} ,x, \bar{x} |
| (13) m x,x,z | (14) m x, \bar{x} ,z | (15) $\bar{4}^+$ 0,0,z; 0,0,0 | (16) $\bar{4}^-$ 0,0,z; 0,0,0 |
| (17) m x,y,y | (18) $\bar{4}^+$ x,0,0; 0,0,0 | (19) $\bar{4}^-$ x,0,0; 0,0,0 | (20) m x,y, \bar{y} |
| (21) m x,y,x | (22) $\bar{4}^-$ 0,y,0; 0,0,0 | (23) m \bar{x} ,y,x | (24) $\bar{4}^+$ 0,y,0; 0,0,0 |

For (0, $\frac{1}{2}$, $\frac{1}{2}$)+ set

- | | | | |
|--|---|--|---|
| (1) $t(0, \frac{1}{2}, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) 0, $\frac{1}{4}$,z | (3) 2(0, $\frac{1}{2}$,0) 0,y, $\frac{1}{4}$ | (4) 2 x, $\frac{1}{4}$, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $-\frac{1}{3}$,x $-\frac{1}{6}$,x | (6) 3 ⁺ \bar{x} ,x $+\frac{1}{2}$, \bar{x} | (7) 3 ⁺ ($-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $+\frac{1}{3}$, $\bar{x}-\frac{1}{6}$, \bar{x} | (8) 3 ⁺ \bar{x} , $\bar{x}+\frac{1}{2}$,x |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $-\frac{1}{6}$,x $+\frac{1}{6}$,x | (10) 3 ⁻ ($-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $+\frac{1}{6}$, $\bar{x}+\frac{1}{6}$, \bar{x} | (11) 3 ⁻ $\bar{x}+\frac{1}{2}$, $\bar{x}+\frac{1}{2}$,x | (12) 3 ⁻ $\bar{x}-\frac{1}{2}$,x $+\frac{1}{2}$, \bar{x} |
| (13) g($\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$) x $-\frac{1}{4}$,x,z | (14) g($-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$) x $+\frac{1}{4}$, \bar{x} ,z | (15) $\bar{4}^+$ $\frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (16) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (17) g(0, $\frac{1}{2}$, $\frac{1}{2}$) x,y,y | (18) $\bar{4}^+$ x, $\frac{1}{2}$,0; 0, $\frac{1}{2}$,0 | (19) $\bar{4}^-$ x,0, $\frac{1}{2}$; 0,0, $\frac{1}{2}$ | (20) m x,y $+\frac{1}{2}$, \bar{y} |
| (21) g($\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$) x $-\frac{1}{4}$,y,x | (22) $\bar{4}^-$ $\frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (23) g($-\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$) $\bar{x}+\frac{1}{4}$,y,x | (24) $\bar{4}^+$ $-\frac{1}{4}, y, \frac{1}{4}; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |

For ($\frac{1}{2}$,0, $\frac{1}{2}$)+ set

- | | | | |
|--|---|---|--|
| (1) $t(\frac{1}{2}, 0, \frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}$,0,z | (3) 2 $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2($\frac{1}{2}$,0,0) x,0, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $+\frac{1}{6}$,x $-\frac{1}{6}$,x | (6) 3 ⁺ ($\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$) $\bar{x}+\frac{1}{6}$,x $+\frac{1}{6}$, \bar{x} | (7) 3 ⁺ x $+\frac{1}{2}$, $\bar{x}-\frac{1}{2}$, \bar{x} | (8) 3 ⁺ $\bar{x}+\frac{1}{2}$, $\bar{x}+\frac{1}{2}$,x |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $-\frac{1}{6}$,x $-\frac{1}{3}$,x | (10) 3 ⁻ x $+\frac{1}{2}$, \bar{x}, \bar{x} | (11) 3 ⁻ $\bar{x}+\frac{1}{2}$, \bar{x}, x | (12) 3 ⁻ ($\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$) $\bar{x}-\frac{1}{6}$,x $+\frac{1}{3}$, \bar{x} |
| (13) g($\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$) x $+\frac{1}{4}$,x,z | (14) g($\frac{1}{4}, -\frac{1}{4}, \frac{1}{2}$) x $+\frac{1}{4}$, \bar{x} ,z | (15) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (16) $\bar{4}^-$ $\frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (17) g($\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$) x,y $-\frac{1}{4}$,y | (18) $\bar{4}^+$ x, $\frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (19) $\bar{4}^-$ x, $-\frac{1}{4}, \frac{1}{4}; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (20) g($\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}$) x,y $+\frac{1}{4}$, \bar{y} |
| (21) g($\frac{1}{2}, 0, \frac{1}{2}$) x,y,x | (22) $\bar{4}^-$ $\frac{1}{2}, y, 0; \frac{1}{2}, 0, 0$ | (23) m $\bar{x}+\frac{1}{2}$,y,x | (24) $\bar{4}^+$ 0,y, $\frac{1}{2}$; 0,0, $\frac{1}{2}$ |

For ($\frac{1}{2}$, $\frac{1}{2}$,0)+ set

- | | | | |
|--|---|---|---|
| (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}$,y,0 | (4) 2($\frac{1}{2}$,0,0) x, $\frac{1}{4}$,0 |
| (5) 3 ⁺ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $+\frac{1}{6}$,x $+\frac{1}{3}$,x | (6) 3 ⁺ $\bar{x}+\frac{1}{2}$,x, \bar{x} | (7) 3 ⁺ x $+\frac{1}{2}$, \bar{x}, \bar{x} | (8) 3 ⁺ ($\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$) $\bar{x}+\frac{1}{6}$, $\bar{x}+\frac{1}{3}$,x |
| (9) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$) x $+\frac{1}{3}$,x $+\frac{1}{6}$,x | (10) 3 ⁻ x, $\bar{x}+\frac{1}{2}$, \bar{x} | (11) 3 ⁻ ($\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}$) $\bar{x}+\frac{1}{3}$, $\bar{x}+\frac{1}{6}$,x | (12) 3 ⁻ $\bar{x}, x+\frac{1}{2}$, \bar{x} |
| (13) g($\frac{1}{2}, \frac{1}{2}, 0$) x,x,z | (14) m x $+\frac{1}{2}$, \bar{x}, z | (15) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$ | (16) $\bar{4}^-$ 0, $\frac{1}{2}, z; 0, \frac{1}{2}, 0$ |
| (17) g($\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$) x,y $+\frac{1}{4}$,y | (18) $\bar{4}^+$ x, $\frac{1}{4}, -\frac{1}{4}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ | (19) $\bar{4}^-$ x, $\frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (20) g($\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}$) x,y $+\frac{1}{4}$, \bar{y} |
| (21) g($\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$) x $+\frac{1}{4}$,y,x | (22) $\bar{4}^-$ $\frac{1}{4}, y, -\frac{1}{4}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ | (23) g($\frac{1}{4}, \frac{1}{2}, -\frac{1}{4}$) $\bar{x}+\frac{1}{4}$,y,x | (24) $\bar{4}^+$ $\frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13)

Positions

	Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions		
		(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+	($\frac{1}{2}$,0, $\frac{1}{2}$)+	($\frac{1}{2}$, $\frac{1}{2}$,0)+	h, k, l permutable		
						General:		
96	<i>i</i> 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) y,x,z (17) x,z,y (21) z,y,x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) \bar{y}, \bar{x}, z (18) \bar{x}, z, \bar{y} (22) z, \bar{y}, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, \bar{z} (19) \bar{x}, \bar{z}, y (23) \bar{z}, y, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, \bar{z} (20) x, \bar{z}, \bar{y} (24) \bar{z}, \bar{y}, x	$hkl : h+k, h+l, k+l = 2n$ $OkI : k, l = 2n$ $hhl : h+l = 2n$ $h00 : h = 2n$		
48	<i>h</i> ..m	x,x,z \bar{z}, \bar{x}, x	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x}	\bar{x}, x, \bar{z} x,z,x	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x}	z,x,x x, \bar{z}, \bar{x}	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x	Special: no extra conditions
24	<i>g</i> 2 .mm	x, $\frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, x$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$	
24	<i>f</i> 2 .mm	x,0,0	$\bar{x}, 0, 0$	0,x,0	0, $\bar{x}, 0$	0,0,x	0,0, \bar{x}	
16	<i>e</i> .3m	x,x,x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}			
4	<i>d</i> $\bar{4}3m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$						
4	<i>c</i> $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$						
4	<i>b</i> $\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						
4	<i>a</i> $\bar{4}3m$	0,0,0						

Symmetry of special projections

Along $[001] p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[111] p31m$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110] c1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** $[2] F231 (F23, 196)$ $(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+$
 $[3] F\bar{4}1m (I\bar{4}m2, 119)$ $(1; 2; 3; 4; 13; 14; 15; 16)+$
 $[3] F\bar{4}1m (I\bar{4}m2, 119)$ $(1; 2; 3; 4; 17; 18; 19; 20)+$
 $[3] F\bar{4}1m (I\bar{4}m2, 119)$ $(1; 2; 3; 4; 21; 22; 23; 24)+$
 $[4] F13m (R3m, 160)$ $(1; 5; 9; 13; 17; 21)+$
 $[4] F13m (R3m, 160)$ $(1; 6; 12; 14; 20; 21)+$
 $[4] F13m (R3m, 160)$ $(1; 7; 10; 14; 17; 23)+$
 $[4] F13m (R3m, 160)$ $(1; 8; 11; 13; 20; 23)+$
- IIa** $[4] P\bar{4}3m (215)$ $1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24$
 $[4] P\bar{4}3m (215)$ $1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + (0, \frac{1}{2}, \frac{1}{2}); (5; 6; 7; 8; 21; 22; 23; 24) + (\frac{1}{2}, 0, \frac{1}{2})$
 $[4] P\bar{4}3m (215)$ $1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + (\frac{1}{2}, 0, \frac{1}{2}); (5; 6; 7; 8; 13; 14; 15; 16) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3m (215)$ $1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + (0, \frac{1}{2}, \frac{1}{2}); (9; 10; 11; 12; 13; 14; 15; 16) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3m (215)$ $1; 5; 9; 13; 17; 21; (4; 6; 11; 15; 20; 22) + (0, \frac{1}{2}, \frac{1}{2}); (3; 8; 10; 16; 18; 23) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 7; 12; 14; 19; 24) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3m (215)$ $1; 6; 12; 14; 20; 21; (4; 5; 10; 16; 17; 22) + (0, \frac{1}{2}, \frac{1}{2}); (3; 7; 11; 15; 19; 23) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 8; 9; 13; 18; 24) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3m (215)$ $1; 7; 10; 14; 17; 23; (4; 8; 12; 16; 20; 24) + (0, \frac{1}{2}, \frac{1}{2}); (3; 6; 9; 15; 18; 21) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 5; 11; 13; 19; 22) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3m (215)$ $1; 8; 11; 13; 20; 23; (4; 7; 9; 15; 17; 24) + (0, \frac{1}{2}, \frac{1}{2}); (3; 5; 12; 16; 19; 21) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 6; 10; 14; 18; 22) + (\frac{1}{2}, \frac{1}{2}, 0)$
- IIb** none

Maximal isomorphic subgroups of lowest index

IIc $[27] F\bar{4}3m (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (216)$

Minimal non-isomorphic supergroups

- I** $[2] Fm\bar{3}m (225); [2] Fd\bar{3}m (227)$
II $[2] P\bar{4}3m (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (215)$

$I\bar{4}3m$

T_d^3

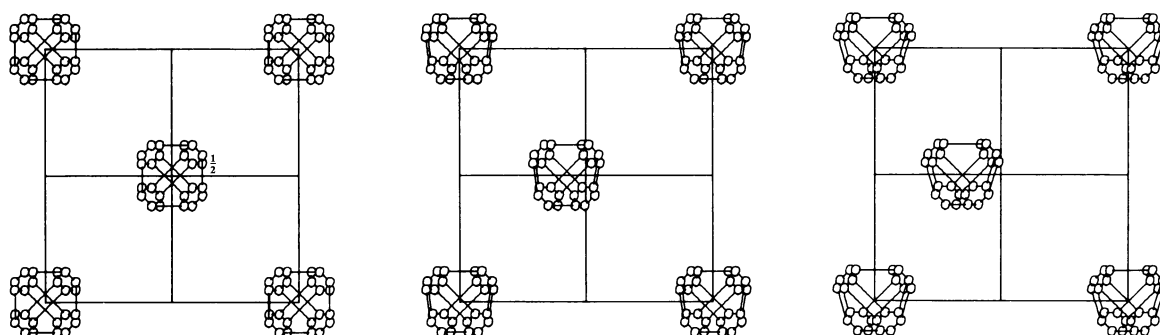
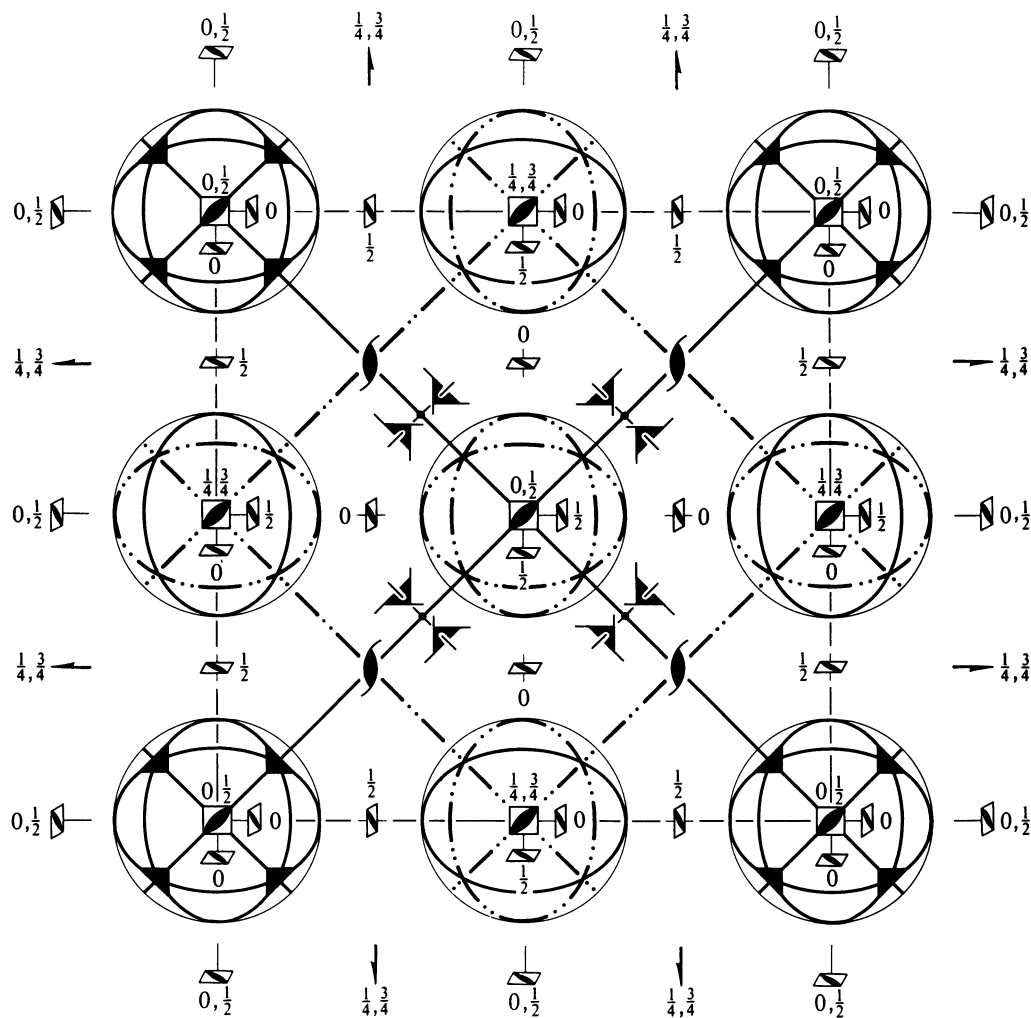
$\bar{4}3m$

Cubic

No. 217

$I\bar{4}3m$

Patterson symmetry $Im\bar{3}m$



Origin at $\bar{4}3m$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq x; z \leq y$
 Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3 ⁺ x,x,x	(6) 3 ⁺ \bar{x} ,x, \bar{x}	(7) 3 ⁺ x, \bar{x} , \bar{x}	(8) 3 ⁺ \bar{x} , \bar{x} ,x
(9) 3 ⁻ x,x,x	(10) 3 ⁻ x, \bar{x} , \bar{x}	(11) 3 ⁻ \bar{x} , \bar{x} ,x	(12) 3 ⁻ \bar{x} ,x, \bar{x}
(13) m x,x,z	(14) m x, \bar{x} ,z	(15) 4 ⁺ 0,0,z; 0,0,0	(16) 4 ⁻ 0,0,z; 0,0,0
(17) m x,y,y	(18) 4 ⁺ x,0,0; 0,0,0	(19) 4 ⁻ x,0,0; 0,0,0	(20) m x,y, \bar{y}
(21) m x,y,x	(22) 4 ⁻ 0,y,0; 0,0,0	(23) m \bar{x} ,y,x	(24) 4 ⁺ 0,y,0; 0,0,0

For ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+ set

(1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}, \frac{1}{4}, z$	(3) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}, y, \frac{1}{4}$	(4) 2($\frac{1}{2}$,0,0) $x, \frac{1}{4}, \frac{1}{4}$
(5) 3 ⁺ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x	(6) 3 ⁺ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$	(7) 3 ⁺ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$	(8) 3 ⁺ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$
(9) 3 ⁻ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x	(10) 3 ⁻ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$	(11) 3 ⁻ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$	(12) 3 ⁻ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$
(13) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,x,z	(14) c $x + \frac{1}{2}, \bar{x}, z$	(15) 4 ⁺ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$	(16) 4 ⁻ 0, $\frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$
(17) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,y,y	(18) 4 ⁺ $x, \frac{1}{2}, 0; \frac{1}{4}, \frac{1}{2}, 0$	(19) 4 ⁻ $x, 0, \frac{1}{2}; \frac{1}{4}, 0, \frac{1}{2}$	(20) a $x, y + \frac{1}{2}, \bar{y}$
(21) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,y,x	(22) 4 ⁻ $\frac{1}{2}, y, 0; \frac{1}{2}, \frac{1}{4}, 0$	(23) b $\bar{x} + \frac{1}{2}, y, x$	(24) 4 ⁺ 0, $y, \frac{1}{2}; 0, \frac{1}{4}, \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (13)**Positions**

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

(0,0,0)+ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+

Reflection conditions

 h, k, l permutable

General:

48	<i>h</i>	1	(1) x,y,z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) z,x,y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}
			(9) y,z,x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x
			(13) y,x,z	(14) \bar{y}, \bar{x}, z	(15) y, \bar{x}, \bar{z}	(16) \bar{y}, x, \bar{z}
			(17) x,z,y	(18) \bar{x}, z, \bar{y}	(19) \bar{x}, \bar{z}, y	(20) x, \bar{z}, \bar{y}
			(21) z,y,x	(22) z, \bar{y}, \bar{x}	(23) \bar{z}, y, \bar{x}	(24) \bar{z}, \bar{y}, x

 $hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$

Special: no extra conditions

24	<i>g</i>	..m	x,x,z \bar{z}, \bar{x}, x	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x}	\bar{x}, x, \bar{z} x,z,x	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x}	z,x,x x, \bar{z}, \bar{x}	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x
24	<i>f</i>	2..	$x, \frac{1}{2}, 0$ $\frac{1}{2}, x, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x}, 0$	0,x, $\frac{1}{2}$ x,0, $\frac{1}{2}$	0, $\bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, x$ 0, $\frac{1}{2}, x$	$\frac{1}{2}, 0, \bar{x}$ 0, $\frac{1}{2}, \bar{x}$
12	<i>e</i>	2.mm	x,0,0	$\bar{x}, 0, 0$	0,x,0	0, $\bar{x}, 0$	0,0,x	0,0, \bar{x}
12	<i>d</i>	4..	$\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, \frac{1}{2}, 0$	0, $\frac{1}{4}, \frac{1}{2}$	0, $\frac{3}{4}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$
8	<i>c</i>	.3m	x,x,x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
6	<i>b</i>	42.m	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	<i>a</i>	43m	0,0,0					

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$

Origin at 0,0,z

Along [111] $p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$

Origin at x,x,x

Along [110] $p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,x,0

(Continued on page 661)

Maximal non-isomorphic subgroups

- I** [2] $I231 (I23, 197)$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
 { [3] $I\bar{4}1m (I\bar{4}2m, 121)$ (1; 2; 3; 4; 13; 14; 15; 16)+
 { [3] $I\bar{4}1m (I\bar{4}2m, 121)$ (1; 2; 3; 4; 17; 18; 19; 20)+
 { [3] $I\bar{4}1m (I\bar{4}2m, 121)$ (1; 2; 3; 4; 21; 22; 23; 24)+
 { [4] $I13m (R3m, 160)$ (1; 5; 9; 13; 17; 21)+
 { [4] $I13m (R3m, 160)$ (1; 6; 12; 14; 20; 21)+
 { [4] $I13m (R3m, 160)$ (1; 7; 10; 14; 17; 23)+
 { [4] $I13m (R3m, 160)$ (1; 8; 11; 13; 20; 23)+
- IIa** [2] $P\bar{4}3n (218)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P\bar{4}3m (215)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [27] $I\bar{4}3m (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (217)$

Minimal non-isomorphic supergroups

- I** [2] $Im\bar{3}m (229)$
II [4] $P\bar{4}3m (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (215)$

$P\bar{4}3n$

T_d^4

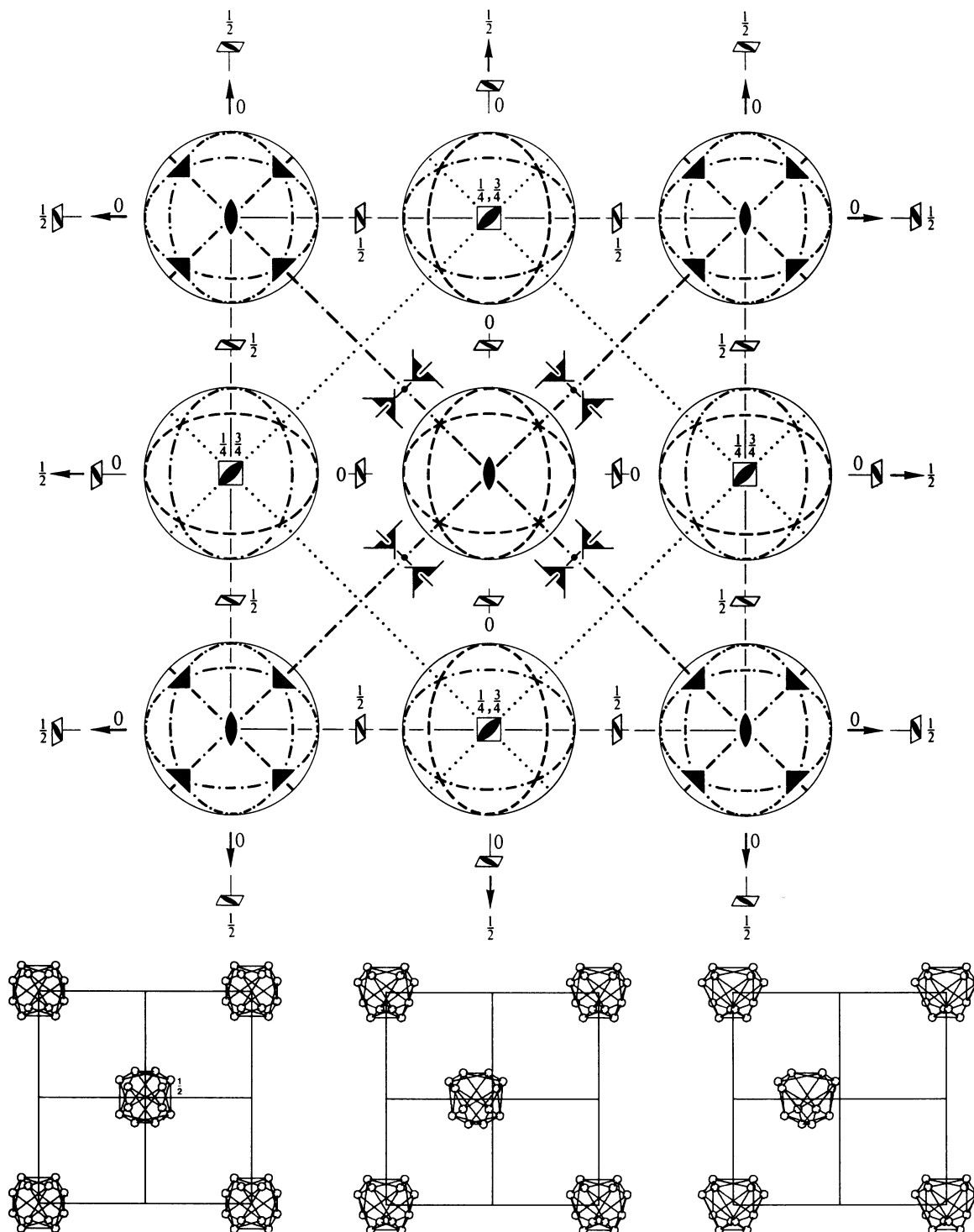
$\bar{4}3m$

Cubic

No. 218

$P\bar{4}3n$

Patterson symmetry $Pm\bar{3}m$



Origin at 23

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; z \leq \min(x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) 3^+ x, x, x | (6) 3^+ \bar{x}, x, \bar{x} | (7) 3^+ x, \bar{x}, \bar{x} | (8) 3^+ \bar{x}, \bar{x}, x |
| (9) 3^- x, x, x | (10) 3^- x, \bar{x}, \bar{x} | (11) 3^- \bar{x}, \bar{x}, x | (12) 3^- \bar{x}, x, \bar{x} |
| (13) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z | (14) c $x + \frac{1}{2}, \bar{x}, z$ | (15) 4^+ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (16) 4^- $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (17) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, y, y | (18) 4^+ $x, \frac{1}{2}, 0; \frac{1}{4}, \frac{1}{2}, 0$ | (19) 4^- $x, 0, \frac{1}{2}; \frac{1}{4}, 0, \frac{1}{2}$ | (20) a $x, y + \frac{1}{2}, \bar{y}$ |
| (21) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, y, x | (22) 4^- $\frac{1}{2}, y, 0; \frac{1}{2}, \frac{1}{4}, 0$ | (23) b $\bar{x} + \frac{1}{2}, y, x$ | (24) 4^+ $0, y, \frac{1}{2}; 0, \frac{1}{4}, \frac{1}{2}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		h, k, l permutable General:
24 <i>i</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{x}, y, \bar{z} (4) x, \bar{y}, \bar{z} (5) z, x, y (6) z, \bar{x}, \bar{y} (7) \bar{z}, \bar{x}, y (8) \bar{z}, x, \bar{y} (9) y, z, x (10) \bar{y}, z, \bar{x} (11) y, \bar{z}, \bar{x} (12) \bar{y}, \bar{z}, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	$hhl : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
12 <i>h</i> 2..	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $\frac{1}{2}, x, 0$ $\frac{1}{2}, \bar{x}, 0$ $0, \frac{1}{2}, x$ $0, \frac{1}{2}, \bar{x}$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, x + \frac{1}{2}$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$hkl : h = 2n$
12 <i>g</i> 2..	$x, \frac{1}{2}, 0$ $\bar{x}, \frac{1}{2}, 0$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, 0, x$ $\frac{1}{2}, 0, \bar{x}$ $0, x + \frac{1}{2}, \frac{1}{2}$ $0, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, x + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x} + \frac{1}{2}$	$hkl : h = 2n$
12 <i>f</i> 2..	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $0, 0, x$ $0, 0, \bar{x}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$
8 <i>e</i> .3.	x, x, x \bar{x}, \bar{x}, x \bar{x}, x, \bar{x} x, \bar{x}, \bar{x} $x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$
6 <i>d</i> $\bar{4}$..	$\frac{1}{4}, 0, \frac{1}{2}$ $\frac{3}{4}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{4}, 0$ $\frac{1}{2}, \frac{3}{4}, 0$ $0, \frac{1}{2}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$
6 <i>c</i> $\bar{4}$..	$\frac{1}{4}, \frac{1}{2}, 0$ $\frac{3}{4}, \frac{1}{2}, 0$ $0, \frac{1}{4}, \frac{1}{2}$ $0, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	
6 <i>b</i> 222..	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : h + k + l = 2n$
2 <i>a</i> 23.	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $\frac{1}{2}, 0, z$	Along [111] $p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x	Along [110] $p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, x, 0$
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Maximal non-isomorphic subgroups

I	[2] $P231$ ($P23, 195$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{	[3] $P\bar{4}1n$ ($P\bar{4}2c, 112$)	1; 2; 3; 4; 13; 14; 15; 16
	[3] $P\bar{4}1n$ ($P\bar{4}2c, 112$)	1; 2; 3; 4; 17; 18; 19; 20
	[3] $P\bar{4}1n$ ($P\bar{4}2c, 112$)	1; 2; 3; 4; 21; 22; 23; 24
	[4] $P13n$ ($R3c, 161$)	1; 5; 9; 13; 17; 21
{	[4] $P13n$ ($R3c, 161$)	1; 6; 12; 14; 20; 21
	[4] $P13n$ ($R3c, 161$)	1; 7; 10; 14; 17; 23
	[4] $P13n$ ($R3c, 161$)	1; 8; 11; 13; 20; 23

IIa none

IIb [4] $I\bar{4}3d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (220)

Maximal isomorphic subgroups of lowest index

IIc [27] $P\bar{4}3n$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (218)

Minimal non-isomorphic supergroups

I [2] $Pn\bar{3}n$ (222); [2] $Pm\bar{3}n$ (223)

II [2] $I\bar{4}3m$ (217); [4] $F\bar{4}3c$ (219)

$F\bar{4}3c$

T_d^5

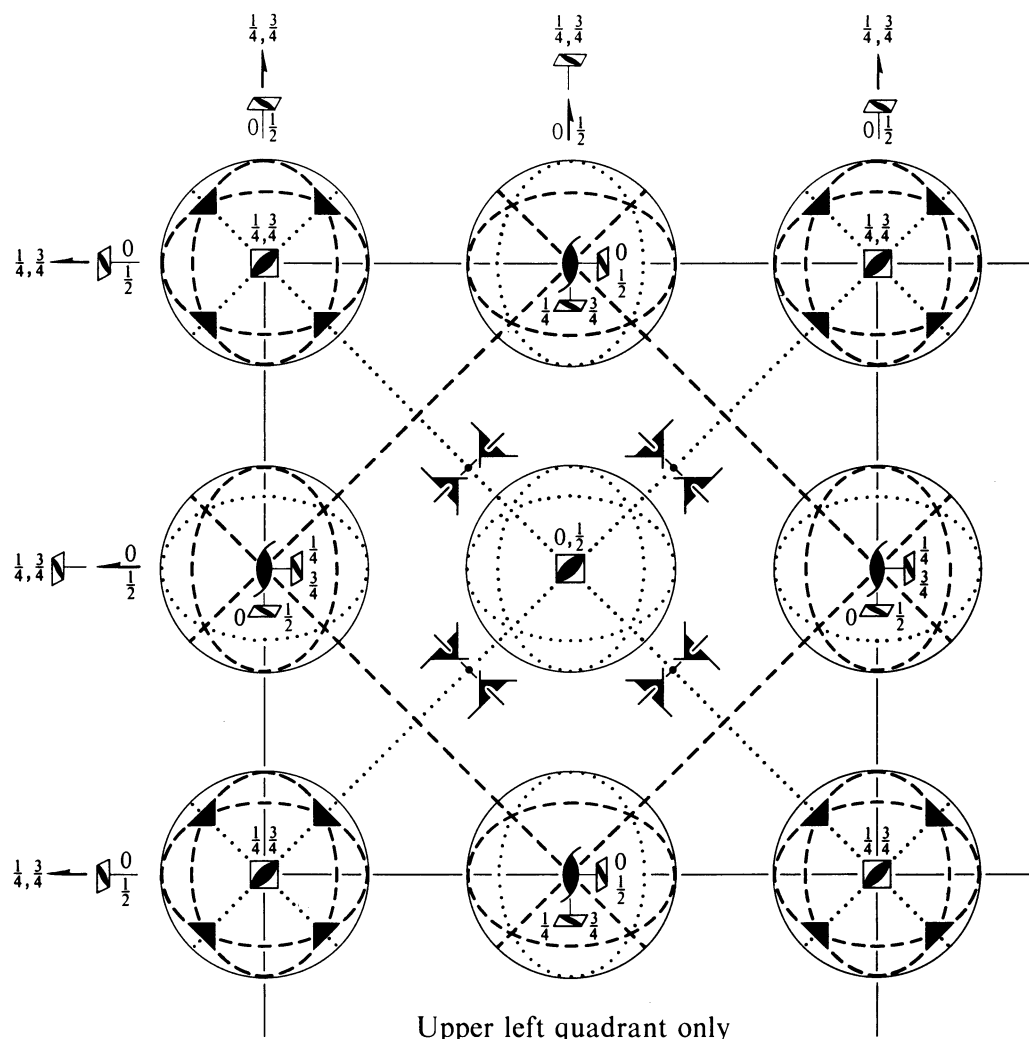
$\bar{4}3m$

Cubic

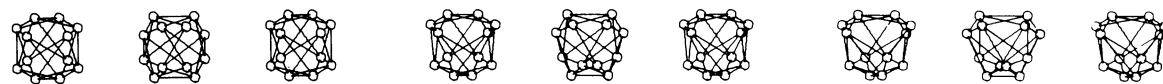
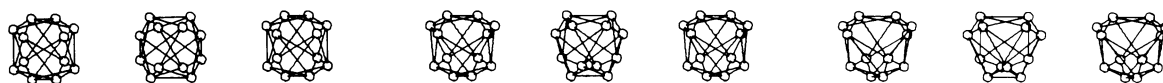
No. 219

$F\bar{4}3c$

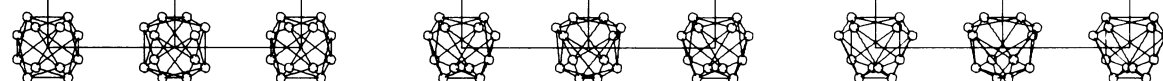
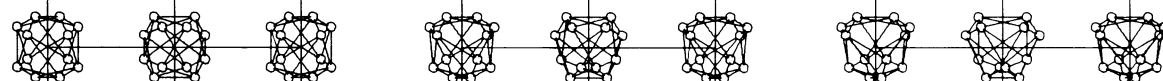
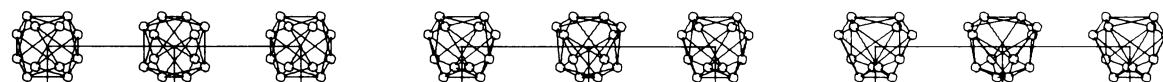
Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Origin at 23

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq \min(x, \frac{1}{2} - x); -y \leq z \leq y$

Vertices $0, 0, 0; \frac{1}{2}, 0, 0; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3 ⁺ x,x,x	(6) 3 ⁺ \bar{x} ,x, \bar{x}	(7) 3 ⁺ x, \bar{x} , \bar{x}	(8) 3 ⁺ \bar{x} , \bar{x} ,x
(9) 3 ⁻ x,x,x	(10) 3 ⁻ x, \bar{x} , \bar{x}	(11) 3 ⁻ \bar{x} , \bar{x} ,x	(12) 3 ⁻ \bar{x} ,x, \bar{x}
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(14) c $x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^-$ $0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(18) $\bar{4}^+$ $x,\frac{1}{2},0; \frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^-$ $x,0,\frac{1}{2}; \frac{1}{4},0,\frac{1}{2}$	(20) a $x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(22) $\bar{4}^-$ $\frac{1}{2},y,0; \frac{1}{2},\frac{1}{4},0$	(23) b $\bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^+$ $0,y,\frac{1}{2}; 0,\frac{1}{4},\frac{1}{2}$

For (0, $\frac{1}{2},\frac{1}{2}$)+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$) 0, $\frac{1}{4},z$	(3) 2(0, $\frac{1}{2},0$) 0,y, $\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x-\frac{1}{3},x-\frac{1}{6},x$	(6) 3 ⁺ $\bar{x},x+\frac{1}{2},\bar{x}$	(7) 3 ⁺ ($-\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) 3 ⁺ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x-\frac{1}{6},x+\frac{1}{6},x$	(10) 3 ⁻ ($-\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) 3 ⁻ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) 3 ⁻ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$	(14) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z; \frac{1}{4},-\frac{1}{4},0$	(16) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},0$
(17) a x,y,y	(18) $\bar{4}^+$ x,0,0; $\frac{1}{4},0,0$	(19) $\bar{4}^-$ x,0,0; $\frac{1}{4},0,0$	(20) a x,y, \bar{y}
(21) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$	(22) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}; \frac{1}{4},0,-\frac{1}{4}$	(23) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}; \frac{1}{4},0,\frac{1}{4}$

For ($\frac{1}{2},0,\frac{1}{2}$)+ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2($\frac{1}{2},0,0$) x,0, $\frac{1}{4}$
(5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x+\frac{1}{6},x-\frac{1}{6},x$	(6) 3 ⁺ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) 3 ⁺ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3 ⁺ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x-\frac{1}{6},x-\frac{1}{3},x$	(10) 3 ⁻ $x+\frac{1}{2},\bar{x},\bar{x}$	(11) 3 ⁻ $\bar{x}+\frac{1}{2},\bar{x},x$	(12) 3 ⁻ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$	(14) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},0$	(16) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z; -\frac{1}{4},\frac{1}{4},0$
(17) $g(0,\frac{1}{4},\frac{1}{4})$ x,y, $\frac{1}{4},y$	(18) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}; 0,\frac{1}{4},-\frac{1}{4}$	(19) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}; 0,\frac{1}{4},\frac{1}{4}$	(20) $g(0,\frac{1}{4},-\frac{1}{4})$ x,y, $\frac{1}{4},\bar{y}$
(21) b x,y,x	(22) $\bar{4}^-$ 0,y,0; 0, $\frac{1}{4},0$	(23) b \bar{x},y,x	(24) $\bar{4}^+$ 0,y,0; 0, $\frac{1}{4},0$

For ($\frac{1}{2},\frac{1}{2},0$)+ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2(0, $\frac{1}{2},0$) $\frac{1}{4},y,0$	(4) 2($\frac{1}{2},0,0$) x, $\frac{1}{4},0$
(5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x+\frac{1}{6},x+\frac{1}{3},x$	(6) 3 ⁺ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3 ⁺ $x+\frac{1}{2},\bar{x},\bar{x}$	(8) 3 ⁺ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) $x+\frac{1}{3},x+\frac{1}{6},x$	(10) 3 ⁻ x, $\bar{x}+\frac{1}{2},\bar{x}$	(11) 3 ⁻ ($\frac{1}{3},\frac{1}{3},-\frac{1}{3}$) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) 3 ⁻ $\bar{x},x+\frac{1}{2},\bar{x}$
(13) c x,x,z	(14) c x, \bar{x},z	(15) $\bar{4}^+$ 0,0,z; 0,0, $\frac{1}{4}$	(16) $\bar{4}^-$ 0,0,z; 0,0, $\frac{1}{4}$
(17) $g(0,\frac{1}{4},\frac{1}{4})$ x,y, $-\frac{1}{4},y$	(18) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}; 0,\frac{1}{4},\frac{1}{4}$	(19) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}; 0,-\frac{1}{4},\frac{1}{4}$	(20) $g(0,-\frac{1}{4},\frac{1}{4})$ x,y, $\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$	(22) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}; \frac{1}{4},0,\frac{1}{4}$	(23) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}; -\frac{1}{4},0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity,	Coordinates				Reflection conditions
Wyckoff letter,					
Site symmetry	(0,0,0)+	(0, $\frac{1}{2},\frac{1}{2}$)+	($\frac{1}{2},0,\frac{1}{2}$)+	($\frac{1}{2},\frac{1}{2},0$)+	<i>h, k, l</i> permutable
					General:

96	<i>h</i>	1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) \bar{x},y,\bar{z}	(4) x, \bar{y},\bar{z}	<i>hkl</i> : <i>h</i> + <i>k</i> = 2 <i>n</i> and <i>h</i> + <i>l</i> , <i>k</i> + <i>l</i> = 2 <i>n</i>
			(5) z,x,y	(6) z, \bar{x},\bar{y}	(7) \bar{z},\bar{x},y	(8) \bar{z},x,\bar{y}	<i>Ok</i> l : <i>k</i> , <i>l</i> = 2 <i>n</i>
			(9) y,z,x	(10) \bar{y},z,\bar{x}	(11) y, \bar{z},\bar{x}	(12) \bar{y},\bar{z},x	<i>hhl</i> : <i>h</i> , <i>l</i> = 2 <i>n</i>
			(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	<i>h00</i> : <i>h</i> = 2 <i>n</i>
			(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	

Special: as above, plus

48	<i>g</i>	2..	$x,\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$ $\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$ $\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	<i>hkl</i> : <i>h</i> = 2 <i>n</i>
48	<i>f</i>	2..	x,0,0 $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	0,x,0 $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	0, $\bar{x},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	0,0,x $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	0,0, \bar{x} $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	<i>hkl</i> : <i>h</i> = 2 <i>n</i>
32	<i>e</i>	.3.	x,x,x $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	\bar{x},\bar{x},x $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	\bar{x},x,\bar{x} $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	x, \bar{x},\bar{x} $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$			<i>hkl</i> : <i>h</i> = 2 <i>n</i>
24	<i>d</i>	$\bar{4}$..	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$	0, $\frac{1}{4},0$	0, $\frac{3}{4},0$	0,0, $\frac{1}{4}$	0,0, $\frac{3}{4}$	<i>hkl</i> : <i>h</i> = 2 <i>n</i>
24	<i>c</i>	$\bar{4}$..	0, $\frac{1}{4},\frac{1}{4}$	0, $\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	<i>hkl</i> : <i>h</i> = 2 <i>n</i>
8	<i>b</i>	23.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					<i>hkl</i> : <i>h</i> = 2 <i>n</i>
8	<i>a</i>	23.	0,0,0	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					<i>hkl</i> : <i>h</i> = 2 <i>n</i>

Symmetry of special projections

Along $[001] p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[111] p31m$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110] p1m1$
 $\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** $[2] F231 (F23, 196)$ $(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+$
 $[3] F\bar{4}1n (I\bar{4}c2, 120)$ $(1; 2; 3; 4; 13; 14; 15; 16)+$
 $[3] F\bar{4}1n (I\bar{4}c2, 120)$ $(1; 2; 3; 4; 17; 18; 19; 20)+$
 $[3] F\bar{4}1n (I\bar{4}c2, 120)$ $(1; 2; 3; 4; 21; 22; 23; 24)+$
 $[4] F13n (R3c, 161)$ $(1; 5; 9; 13; 17; 21)+$
 $[4] F13n (R3c, 161)$ $(1; 6; 12; 14; 20; 21)+$
 $[4] F13n (R3c, 161)$ $(1; 7; 10; 14; 17; 23)+$
 $[4] F13n (R3c, 161)$ $(1; 8; 11; 13; 20; 23)+$
- IIa** $[4] P\bar{4}3n (218)$ $1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24$
 $[4] P\bar{4}3n (218)$ $1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + (0, \frac{1}{2}, \frac{1}{2}); (5; 6; 7; 8; 21; 22; 23; 24) + (\frac{1}{2}, 0, \frac{1}{2})$
 $[4] P\bar{4}3n (218)$ $1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + (\frac{1}{2}, 0, \frac{1}{2}); (5; 6; 7; 8; 13; 14; 15; 16) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3n (218)$ $1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + (0, \frac{1}{2}, \frac{1}{2}); (9; 10; 11; 12; 13; 14; 15; 16) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3n (218)$ $1; 5; 9; 13; 17; 21; (4; 6; 11; 15; 20; 22) + (0, \frac{1}{2}, \frac{1}{2}); (3; 8; 10; 16; 18; 23) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 7; 12; 14; 19; 24) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3n (218)$ $1; 6; 12; 14; 20; 21; (4; 5; 10; 16; 17; 22) + (0, \frac{1}{2}, \frac{1}{2}); (3; 7; 11; 15; 19; 23) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 8; 9; 13; 18; 24) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3n (218)$ $1; 7; 10; 14; 17; 23; (4; 8; 12; 16; 20; 24) + (0, \frac{1}{2}, \frac{1}{2}); (3; 6; 9; 15; 18; 21) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 5; 11; 13; 19; 22) + (\frac{1}{2}, \frac{1}{2}, 0)$
 $[4] P\bar{4}3n (218)$ $1; 8; 11; 13; 20; 23; (4; 7; 9; 15; 17; 24) + (0, \frac{1}{2}, \frac{1}{2}); (3; 5; 12; 16; 19; 21) + (\frac{1}{2}, 0, \frac{1}{2}); (2; 6; 10; 14; 18; 22) + (\frac{1}{2}, \frac{1}{2}, 0)$
- IIb** none

Maximal isomorphic subgroups of lowest index

IIc $[27] F\bar{4}3c (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (219)$

Minimal non-isomorphic supergroups

- I** $[2] Fm\bar{3}c (226); [2] Fd\bar{3}c (228)$
II $[2] P\bar{4}3m (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (215)$

$I\bar{4}3d$

T_d^6

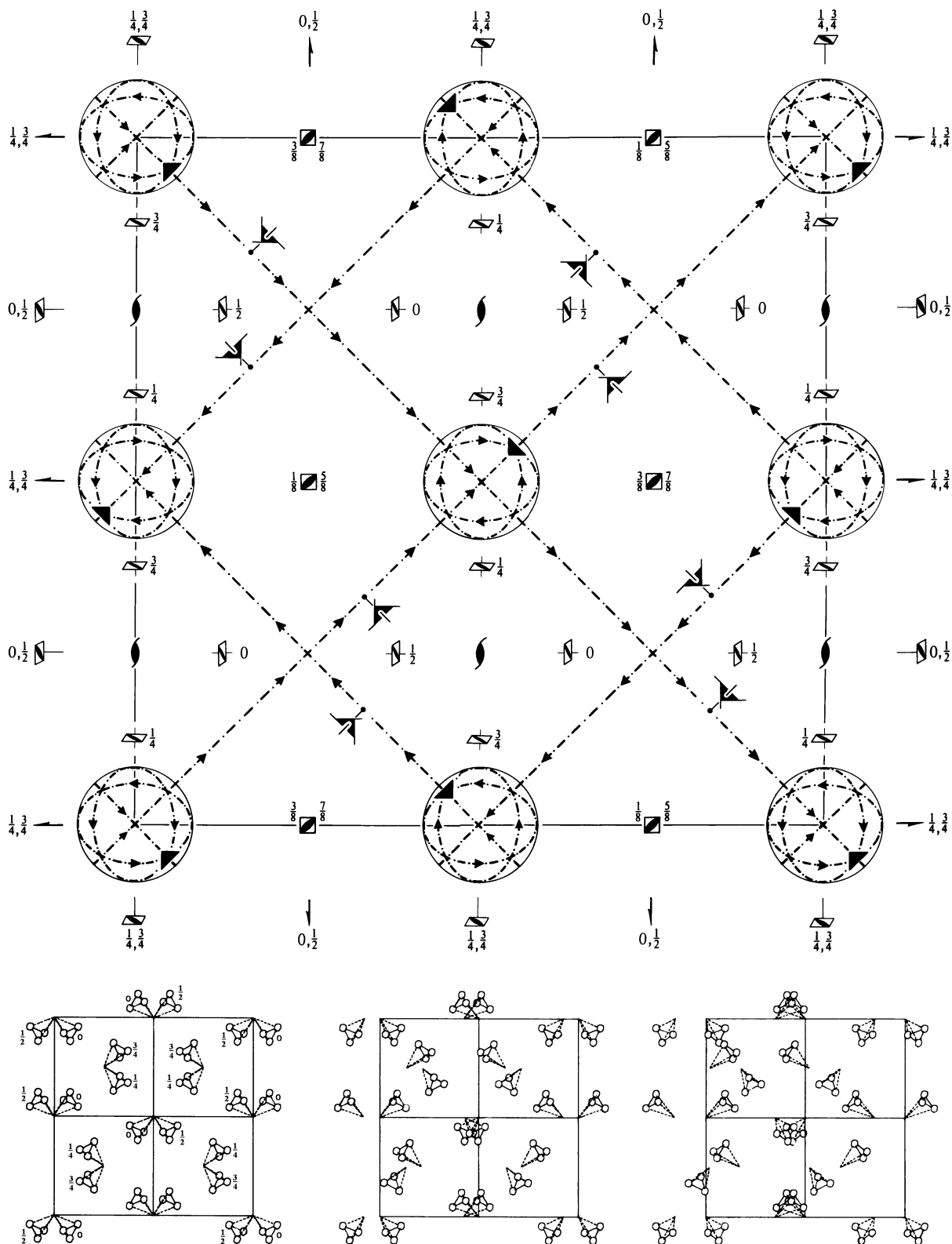
$\bar{4}3m$

Cubic

No. 220

$I\bar{4}3d$

Patterson symmetry $Im\bar{3}m$



Origin on $3[111]$ at midpoint of three non-intersecting pairs of parallel $\bar{4}$ axes and of three non-intersecting pairs of parallel 2_2 axes

Asymmetric unit $\frac{1}{4} \leq x \leq \frac{1}{2}; \frac{1}{4} \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; z \leq \min(x, y)$

Vertices $\frac{1}{4}, \frac{1}{4}, 0 \quad \frac{1}{2}, \frac{1}{4}, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{2}, 0$
 $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{2}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \quad \frac{1}{4}, \frac{1}{2}, \frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---|--|--|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},0,z$ | (3) $2(0,\frac{1}{2},0) \quad 0,y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},0$ |
| (5) $3^+ x,x,x$ | (6) $3^+ \bar{x}+\frac{1}{2},x,\bar{x}$ | (7) $3^+ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+ \bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) $3^- x,x,x$ | (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3}) \quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^-(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3}) \quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^-(-\frac{1}{3},-\frac{1}{3},\frac{1}{3}) \quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4}) \quad x,x,z$ | (14) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4}) \quad x+\frac{1}{2},\bar{x},z$ | (15) $\bar{4}^+ \frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ | (16) $\bar{4}^- 0,\frac{3}{4},z; 0,\frac{3}{4},\frac{1}{8}$ |
| (17) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4}) \quad x,y,y$ | (18) $\bar{4}^+ x,\frac{1}{2},-\frac{1}{4}; \frac{3}{8},\frac{1}{2},-\frac{1}{4}$ | (19) $\bar{4}^- x,0,\frac{3}{4}; \frac{1}{8},0,\frac{3}{4}$ | (20) $d(\frac{3}{4},-\frac{1}{4},\frac{1}{4}) \quad x,y+\frac{1}{2},\bar{y}$ |
| (21) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4}) \quad x,y,x$ | (22) $\bar{4}^- \frac{3}{4},y,0; \frac{3}{4},\frac{1}{8},0$ | (23) $d(\frac{1}{4},\frac{3}{4},-\frac{1}{4}) \quad \bar{x}+\frac{1}{2},y,x$ | (24) $\bar{4}^+ -\frac{1}{4},y,\frac{1}{2}; -\frac{1}{4},\frac{3}{8},\frac{1}{2}$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

- | | | | |
|--|---|--|--|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2 \quad 0,\frac{1}{4},z$ | (3) $2 \quad \frac{1}{4},y,0$ | (4) $2 \quad x,0,\frac{1}{4}$ |
| (5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2}) \quad x,x,x$ | (6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6}) \quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ | (7) $3^+(\frac{1}{6},\frac{1}{6},\frac{1}{6}) \quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6}) \quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{6},x$ |
| (9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2}) \quad x,x,x$ | (10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6}) \quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6}) \quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6}) \quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \quad x,x,z$ | (14) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) \quad x+\frac{1}{2},\bar{x},z$ | (15) $\bar{4}^+ \frac{1}{2},\frac{1}{4},z; \frac{1}{2},\frac{1}{4},\frac{1}{8}$ | (16) $\bar{4}^- 0,\frac{1}{4},z; 0,\frac{1}{4},\frac{3}{8}$ |
| (17) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \quad x,y,y$ | (18) $\bar{4}^+ x,\frac{1}{2},\frac{1}{4}; \frac{1}{8},\frac{1}{2},\frac{1}{4}$ | (19) $\bar{4}^- x,0,\frac{1}{4}; \frac{3}{8},0,\frac{1}{4}$ | (20) $d(\frac{1}{4},\frac{1}{4},-\frac{1}{4}) \quad x,y+\frac{1}{2},\bar{y}$ |
| (21) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \quad x,y,x$ | (22) $\bar{4}^- \frac{1}{4},y,0; \frac{1}{4},\frac{3}{8},0$ | (23) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4}) \quad \bar{x}+\frac{1}{2},y,x$ | (24) $\bar{4}^+ \frac{1}{4},y,\frac{1}{2}; \frac{1}{4},\frac{1}{8},\frac{1}{2}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity,	Coordinates	Reflection conditions
Wyckoff letter,		
Site symmetry	$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	h,k,l permutable

- | | | | | | | |
|----|-------------|--|--|--|--|---|
| 48 | $e \quad 1$ | (1) x,y,z | (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ | (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ | (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ | $hkl : h+k+l=2n$
$OkI : k+l=2n$
$hhl : 2h+l=4n$
$h00 : h=4n$ |
| | | (5) z,x,y | (6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$ | (7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$ | (8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$ | |
| | | (9) y,z,x | (10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$ | (11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$ | (12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$ | |
| | | (13) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$ | (14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$ | (15) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$ | (16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$ | |
| | | (17) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$ | (18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$ | (19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$ | (20) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$ | |
| | | (21) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$ | (22) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$ | (23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$ | (24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$ | |

Special: as above, plus

- | | | | | | | | | |
|----|---------------------|---|---|---|---|--|-------------------------------------|-----------------------------|
| 24 | $d \quad 2..$ | $x,0,\frac{1}{4}$ | $\bar{x}+\frac{1}{2},0,\frac{3}{4}$ | $\frac{1}{4},x,0$ | $\frac{3}{4},\bar{x}+\frac{1}{2},0$ | $0,\frac{1}{4},x$ | $0,\frac{3}{4},\bar{x}+\frac{1}{2}$ | $hkl : h=2n+1$
or $h=4n$ |
| | | $\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$ | $\frac{1}{4},\bar{x}+\frac{3}{4},0$ | $x+\frac{1}{4},\frac{1}{2},\frac{1}{4}$ | $\bar{x}+\frac{3}{4},0,\frac{1}{4}$ | $\frac{1}{2},\frac{1}{4},x+\frac{1}{4}$ | $0,\frac{1}{4},\bar{x}+\frac{3}{4}$ | |
| 16 | $c \quad .3.$ | x,x,x | $\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$ | $\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ | $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$ | $hkl : h=2n+1$
or $h+k+l=4n$ | | |
| | | $x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$ | $\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$ | $x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$ | $\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$ | | | |
| 12 | $b \quad \bar{4}..$ | $\frac{7}{8},0,\frac{1}{4}$ | $\frac{5}{8},0,\frac{3}{4}$ | $\frac{1}{4},\frac{7}{8},0$ | $\frac{3}{4},\frac{5}{8},0$ | $hkl : h,k=2n, h+k+l=4n$
or $h,k=2n+1, l=4n+2$
or $h=8n, k=8n+4$ and
$h+k+l=4n+2$
or $h=8n+1$ and
$k=8n+3, l=4n$
or $h=8n+1$ and
$k=8n+5, l=4n$
or $h=8n+7$ and
$k=8n+3, l=4n$
or $h=8n+7$ and
$k=8n+5, l=4n$ | | |
| 12 | $a \quad \bar{4}..$ | $\frac{3}{8},0,\frac{1}{4}$ | $\frac{1}{8},0,\frac{3}{4}$ | $\frac{1}{4},\frac{3}{8},0$ | $\frac{3}{4},\frac{1}{8},0$ | | | |
| | | $0,\frac{1}{4},\frac{7}{8}$ | $0,\frac{3}{4},\frac{5}{8}$ | $0,\frac{1}{4},\frac{3}{8}$ | $0,\frac{3}{4},\frac{1}{8}$ | | | |

Symmetry of special projections

Along [001] $p4gm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0,\frac{1}{4},z$

(Continued on page 669)

Along [111] $p31m$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x,x,x Along [110] $c1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x,x+\frac{1}{4},0$

Maximal non-isomorphic subgroups

- I** [2] $I2_131(I2_13, 199)$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
 { [3] $I\bar{4}1d(I\bar{4}2d, 122)$ (1; 2; 3; 4; 13; 14; 15; 16)+
 [3] $I\bar{4}1d(I\bar{4}2d, 122)$ (1; 2; 3; 4; 17; 18; 19; 20)+
 [3] $I\bar{4}1d(I\bar{4}2d, 122)$ (1; 2; 3; 4; 21; 22; 23; 24)+
 { [4] $I13d(R3c, 161)$ (1; 5; 9; 13; 17; 21)+
 [4] $I13d(R3c, 161)$ (1; 6; 12; 14; 20; 21)+
 [4] $I13d(R3c, 161)$ (1; 7; 10; 14; 17; 23)+
 [4] $I13d(R3c, 161)$ (1; 8; 11; 13; 20; 23)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $I\bar{4}3d(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c})$ (220)

Minimal non-isomorphic supergroups

I [2] $Ia\bar{3}d$ (230)

II [4] $P\bar{4}3n(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})$ (218)

$Pm\bar{3}m$

O_h^1

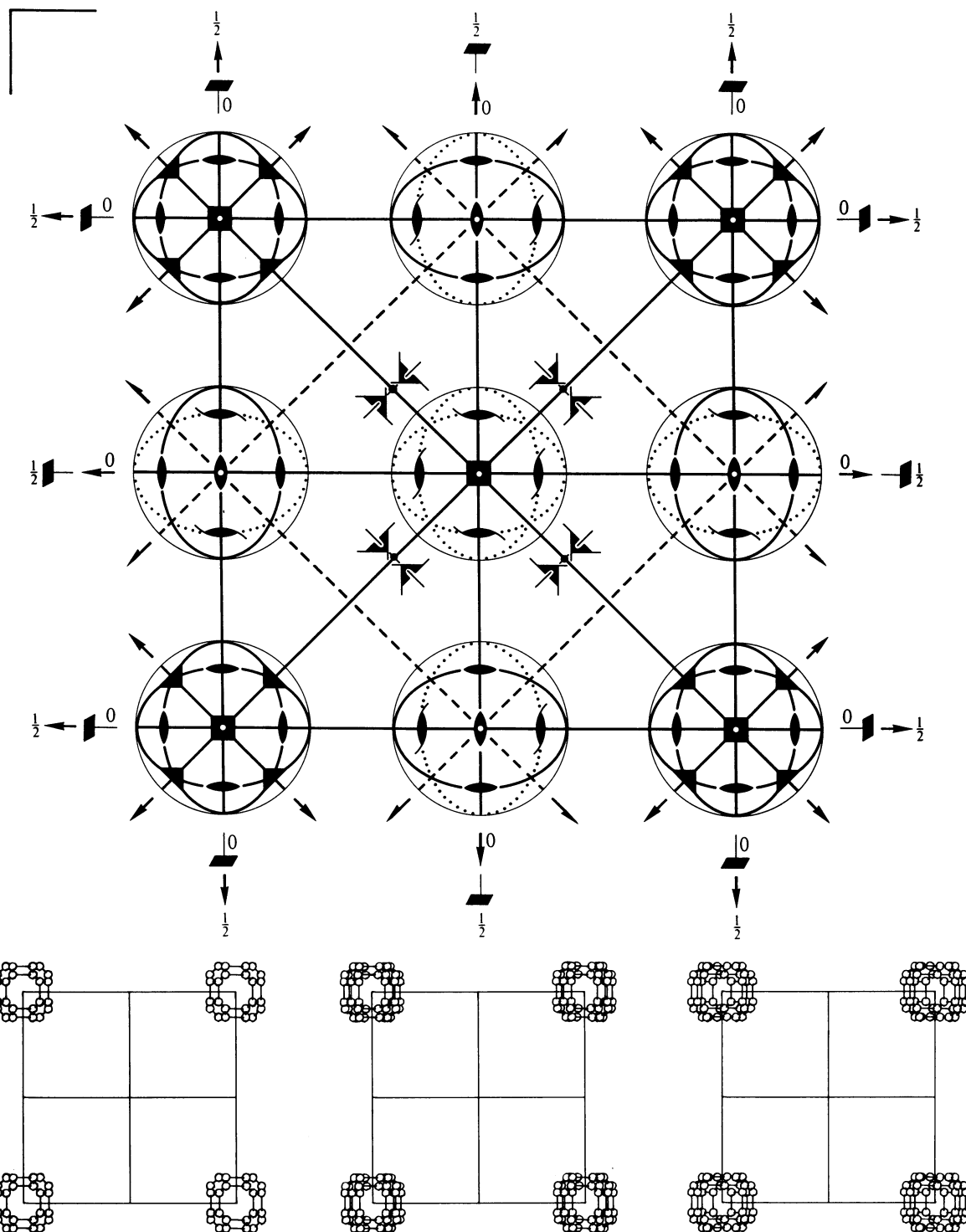
$m\bar{3}m$

Cubic

No. 221

$P 4/m \bar{3} 2/m$

Patterson symmetry $Pm\bar{3}m$



Origin at centre ($m\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq x; z \leq y$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(given on page 674)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
								h, k, l permutable
								General:
48	n 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) y, x, \bar{z} (17) x, z, \bar{y} (21) z, y, \bar{x} (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) \bar{y}, \bar{x}, z (41) \bar{x}, \bar{z}, y (45) \bar{z}, \bar{y}, x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y}, \bar{x}, \bar{z}$ (18) \bar{x}, z, y (22) z, \bar{y}, x (26) x, y, \bar{z} (30) \bar{z}, x, y (34) y, \bar{z}, x (38) y, x, z (42) x, \bar{z}, \bar{y} (46) \bar{z}, y, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, z (19) $\bar{x}, \bar{z}, \bar{y}$ (23) \bar{z}, y, x (27) x, \bar{y}, z (31) z, x, \bar{y} (35) \bar{y}, z, x (39) \bar{y}, x, \bar{z} (43) x, z, y (47) z, \bar{y}, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, z (20) x, \bar{z}, y (24) $\bar{z}, \bar{y}, \bar{x}$ (28) \bar{x}, y, z (32) z, \bar{x}, y (36) y, z, \bar{x} (40) y, \bar{x}, \bar{z} (44) \bar{x}, z, \bar{y} (48) z, y, x			no conditions
24	m . . m	x, x, z \bar{z}, \bar{x}, x x, x, \bar{z} $\bar{x}, \bar{z}, \bar{x}$	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x} $\bar{x}, \bar{x}, \bar{z}$ x, \bar{z}, x	\bar{x}, x, \bar{z} x, z, x x, \bar{x}, z z, x, \bar{x}	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x} \bar{x}, x, z z, \bar{x}, x	z, x, x x, \bar{z}, \bar{x} x, z, \bar{x} \bar{z}, x, x	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x \bar{x}, z, x $\bar{z}, \bar{x}, \bar{x}$	Special: no extra conditions
24	l m . .	$\frac{1}{2}, y, z$ $\bar{z}, \frac{1}{2}, y$ $y, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \bar{z}, \bar{y}$	$\frac{1}{2}, \bar{y}, z$ $\bar{z}, \frac{1}{2}, \bar{y}$ $\bar{y}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \bar{z}, y$	$\frac{1}{2}, y, \bar{z}$ $y, z, \frac{1}{2}$ $y, \frac{1}{2}, z$ $z, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{z}$ $\bar{y}, z, \frac{1}{2}$ $\bar{y}, \frac{1}{2}, z$ $z, \bar{y}, \frac{1}{2}$	$z, \frac{1}{2}, y$ $y, \bar{z}, \frac{1}{2}$ $\frac{1}{2}, z, \bar{y}$ $\bar{z}, y, \frac{1}{2}$	$z, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{z}, \frac{1}{2}$ $\frac{1}{2}, z, y$ $\bar{z}, \bar{y}, \frac{1}{2}$	
24	k m . .	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	
12	j m . $m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	
12	i m . $m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	
12	h m $m2$. .	$x, \frac{1}{2}, 0$ $\frac{1}{2}, x, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x}, 0$	$0, x, \frac{1}{2}$ $x, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, x$ $0, \frac{1}{2}, \bar{x}$	$\frac{1}{2}, 0, \bar{x}$ $0, \frac{1}{2}, x$	
8	g . $3m$	x, x, x x, x, \bar{x}	\bar{x}, \bar{x}, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x			
6	f $4m$. m	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$	
6	e $4m$. m	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	
3	d $4/m$ m . m	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$				
3	c $4/m$ m . m	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$				
1	b $m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						
1	a $m\bar{3}m$	$0, 0, 0$						

Symmetry of special projections

Along $[001]$ $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along $[111]$ $p6mm$
 $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pm\bar{3}1$ ($Pm\bar{3}$, 200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4/m12/m(P4/mmm, 123)$	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4/m12/m(P4/mmm, 123)$	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4/m12/m(P4/mmm, 123)$	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb [2] $Fm\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (226); [2] $Fm\bar{3}m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (225); [4] $Im\bar{3}m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (229)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pm\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (221)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

Symmetry operations

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3 ⁺ x,x,x	(6) 3 ⁺ \bar{x},x,\bar{x}	(7) 3 ⁺ x, \bar{x},\bar{x}	(8) 3 ⁺ \bar{x},\bar{x},x
(9) 3 ⁻ x,x,x	(10) 3 ⁻ x, \bar{x},\bar{x}	(11) 3 ⁻ \bar{x},\bar{x},x	(12) 3 ⁻ \bar{x},x,\bar{x}
(13) 2 x,x,0	(14) 2 x, $\bar{x},0$	(15) 4 ⁻ 0,0,z	(16) 4 ⁺ 0,0,z
(17) 4 ⁻ x,0,0	(18) 2 0,y,y	(19) 2 0,y, \bar{y}	(20) 4 ⁺ x,0,0
(21) 4 ⁺ 0,y,0	(22) 2 x,0,x	(23) 4 ⁻ 0,y,0	(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ 0,0,0	(26) m x,y,0	(27) m x,0,z	(28) m 0,y,z
(29) 3 ⁺ x,x,x; 0,0,0	(30) 3 ⁺ $\bar{x},x,\bar{x}; 0,0,0$	(31) 3 ⁺ x, $\bar{x},\bar{x}; 0,0,0$	(32) 3 ⁺ $\bar{x},\bar{x},x; 0,0,0$
(33) 3 ⁻ x,x,x; 0,0,0	(34) 3 ⁻ x, $\bar{x},\bar{x}; 0,0,0$	(35) 3 ⁻ $\bar{x},\bar{x},x; 0,0,0$	(36) 3 ⁻ $\bar{x},x,\bar{x}; 0,0,0$
(37) m x, \bar{x},z	(38) m x,x,z	(39) 4 ⁻ 0,0,z; 0,0,0	(40) 4 ⁺ 0,0,z; 0,0,0
(41) 4 ⁻ x,0,0; 0,0,0	(42) m x,y, \bar{y}	(43) m x,y,y	(44) 4 ⁺ x,0,0; 0,0,0
(45) 4 ⁺ 0,y,0; 0,0,0	(46) m \bar{x},y,x	(47) 4 ⁻ 0,y,0; 0,0,0	(48) m x,y,x

$Pn\bar{3}n$

O_h^2

$m\bar{3}m$

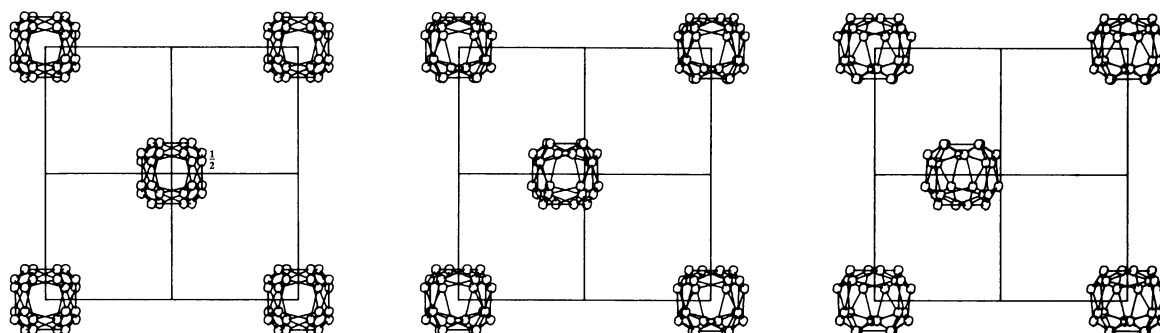
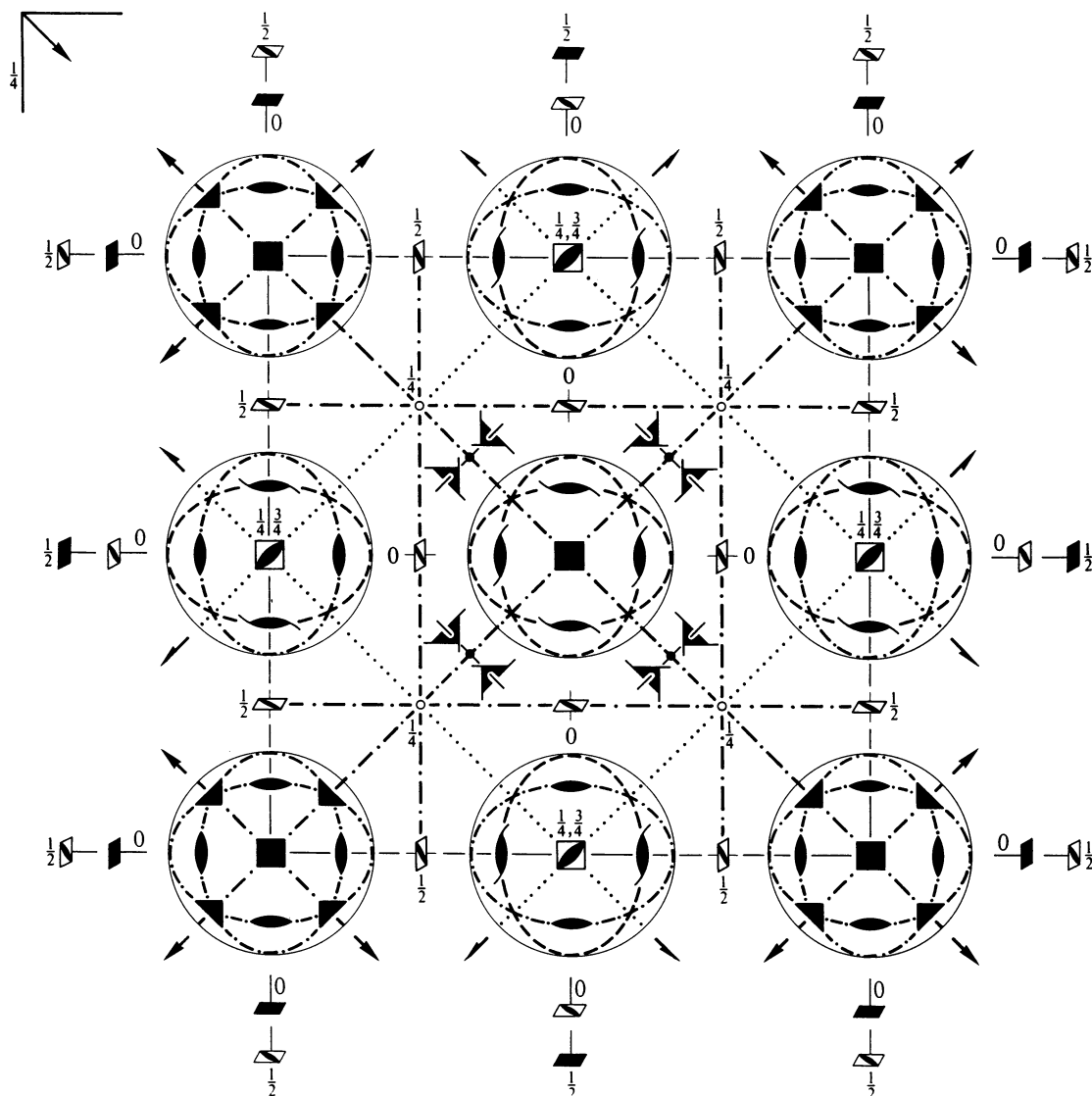
Cubic

No. 222

$P 4/n \bar{3} 2/n$

Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1



Origin at 432, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq x; z \leq y$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3 ⁺ x,x,x	(6) 3 ⁺ \bar{x} ,x, \bar{x}	(7) 3 ⁺ x, \bar{x} , \bar{x}	(8) 3 ⁺ \bar{x} , \bar{x} ,x
(9) 3 ⁻ x,x,x	(10) 3 ⁻ x, \bar{x} , \bar{x}	(11) 3 ⁻ \bar{x} , \bar{x} ,x	(12) 3 ⁻ \bar{x} ,x, \bar{x}
(13) 2 x,x,0	(14) 2 x, \bar{x} ,0	(15) 4 ⁻ 0,0,z	(16) 4 ⁺ 0,0,z
(17) 4 ⁻ x,0,0	(18) 2 0,y,y	(19) 2 0,y, \bar{y}	(20) 4 ⁺ x,0,0
(21) 4 ⁺ 0,y,0	(22) 2 x,0,x	(23) 4 ⁻ 0,y,0	(24) 2 \bar{x} ,0,x
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(26) $n(\frac{1}{2},\frac{1}{2},0)$ x,y, $\frac{1}{4}$	(27) $n(\frac{1}{2},0,\frac{1}{2})$ x, $\frac{1}{4}$,z	(28) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4}$,y,z
(29) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{4},\frac{3}{4},\frac{3}{4}$	(31) $\bar{3}^+$ x, $\bar{x}+1,\bar{x}$; $\frac{3}{4},\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(34) $\bar{3}^-$ x+1, $\bar{x}-1,\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) c x+ $\frac{1}{2}$, \bar{x} ,z	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(39) $\bar{4}^-$ 0, $\frac{1}{2}$,z; 0, $\frac{1}{2}$, $\frac{1}{4}$	(40) $\bar{4}^+$ $\frac{1}{2}$,0,z; $\frac{1}{2}$,0, $\frac{1}{4}$
(41) $\bar{4}^-$ x,0, $\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$	(42) a x,y+ $\frac{1}{2}$, \bar{y}	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(44) $\bar{4}^+$ x, $\frac{1}{2}$,0; $\frac{1}{4},\frac{1}{2}$,0
(45) $\bar{4}^+$ 0,y, $\frac{1}{2}$; 0, $\frac{1}{4},\frac{1}{2}$	(46) b $\bar{x}+\frac{1}{2}$,y,x	(47) $\bar{4}^-$ $\frac{1}{2}$,y,0; $\frac{1}{2},\frac{1}{4},0$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

Reflection conditions

 h, k, l permutable

General:

48	<i>i</i>	1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) \bar{x},y,\bar{z}	(4) x, \bar{y},\bar{z}	$0kl : k+l=2n$
			(5) z,x,y	(6) z, \bar{x},\bar{y}	(7) \bar{z},\bar{x},y	(8) \bar{z},x,\bar{y}	$hhl : l=2n$
			(9) y,z,x	(10) \bar{y},z,\bar{x}	(11) y, \bar{z},\bar{x}	(12) \bar{y},\bar{z},x	$h00 : h=2n$
			(13) y,x, \bar{z}	(14) \bar{y},\bar{x},\bar{z}	(15) y, \bar{x},z	(16) \bar{y},x,z	
			(17) x,z, \bar{y}	(18) \bar{x},z,y	(19) \bar{x},\bar{z},\bar{y}	(20) x, \bar{z},y	
			(21) z,y, \bar{x}	(22) z, \bar{y},x	(23) \bar{z},y,x	(24) \bar{z},\bar{y},\bar{x}	
			(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	
			(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	

Special: as above, plus

24	<i>h</i>	..2	0,y,y	0, \bar{y},y	0,y, \bar{y}	0, \bar{y},\bar{y}	$hkl : h+k+l=2n$
			y,0,y	y,0, \bar{y}	$\bar{y},0,y$	$\bar{y},0,\bar{y}$	
			y,y,0	$\bar{y},\bar{y},0$	y, $\bar{y},0$	$\bar{y},\bar{y},0$	
			$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},y+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},y+\frac{1}{2}$	
			$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},y+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},\bar{y}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},y+\frac{1}{2}$	
			$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	

24	<i>g</i>	2..	x,0, $\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	0, $\frac{1}{2},x$	0, $\frac{1}{2},\bar{x}$	$hkl : h+k+l=2n$
			0,x, $\frac{1}{2}$	0, $\bar{x},\frac{1}{2}$	x, $\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},0,\bar{x}$	$\frac{1}{2},0,x$	
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	0, $\bar{x}+\frac{1}{2},\frac{1}{2}$	0,x+ $\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\bar{x}+\frac{1}{2}$	$\frac{1}{2},0,x+\frac{1}{2}$	
			$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$	0, $\frac{1}{2},x+\frac{1}{2}$	0, $\frac{1}{2},\bar{x}+\frac{1}{2}$	

16	<i>f</i>	.3.	x,x,x	\bar{x},\bar{x},x	\bar{x},x,\bar{x}	x, \bar{x},\bar{x}	$hkl : h+k+l=2n$
			x,x, \bar{x}	\bar{x},\bar{x},\bar{x}	x, \bar{x},x	\bar{x},x,x	
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	

12	<i>e</i>	4..	x,0,0	$\bar{x},0,0$	0,x,0	0, $\bar{x},0$	0,0,x	0,0, \bar{x}	$hkl : h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	

12	<i>d</i>	$\bar{4}..$	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	0, $\frac{1}{2},\frac{1}{4}$	0, $\frac{1}{2},\frac{3}{4}$	$hkl : h+k+l=2n$
			0, $\frac{1}{4},\frac{1}{2}$	0, $\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	

8	<i>c</i>	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$hkl : h,k,l=2n$
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6	<i>b</i>	42.2	0, $\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	0, $\frac{1}{2},0$	0,0, $\frac{1}{2}$	$hkl : h+k+l=2n$
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2	<i>a</i>	432	0,0,0	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					$hkl : h+k+l=2n$
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(Continued on page 675)

ORIGIN CHOICE 1

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[111]$ $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

ORIGIN CHOICE 2

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along $[111]$ $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}n$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (222)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

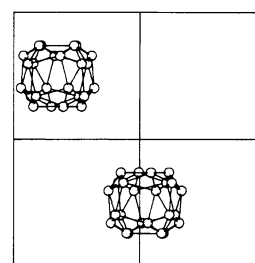
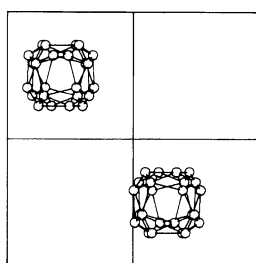
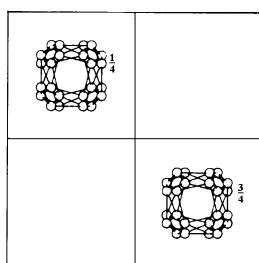
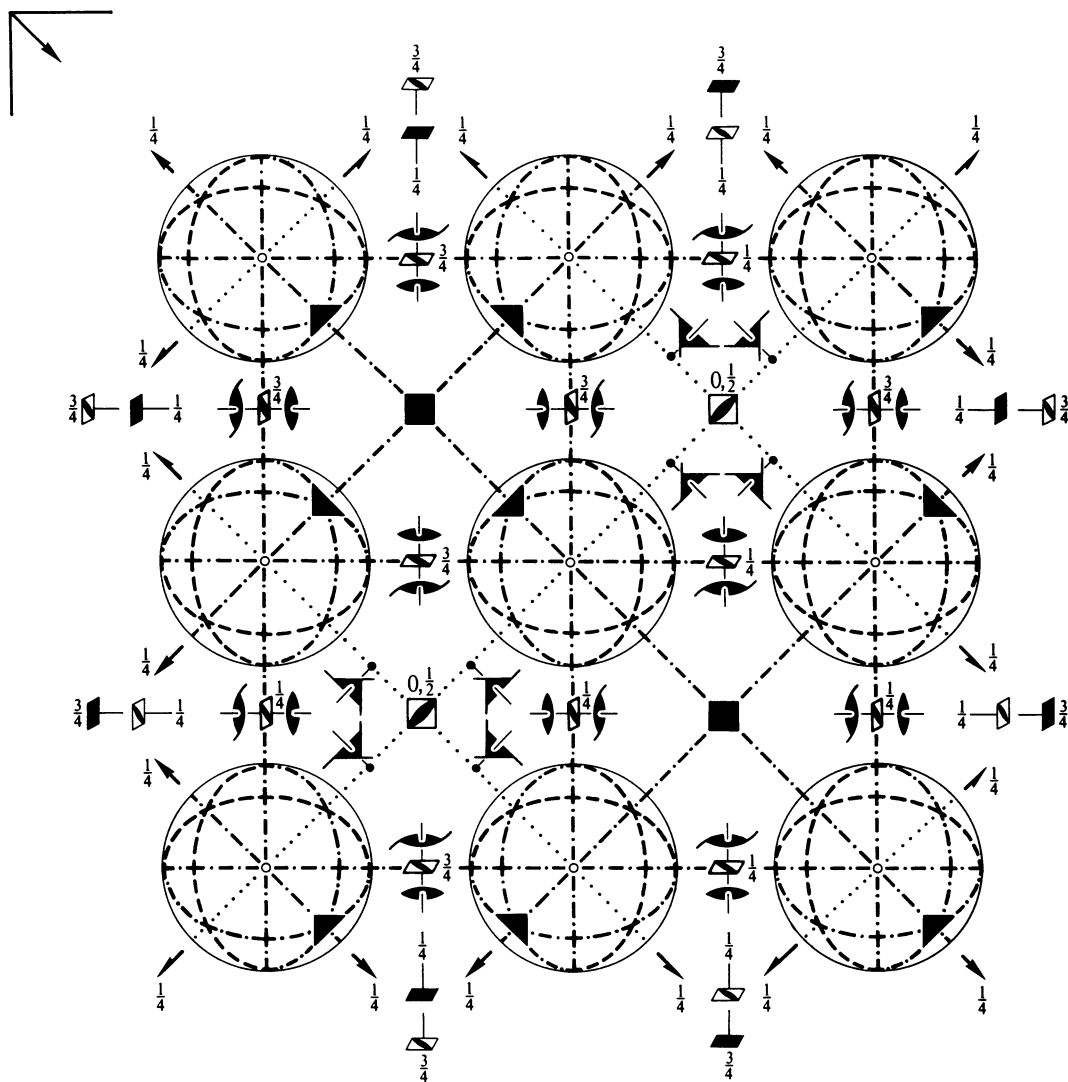
$Pn\bar{3}n$ O_h^2 $m\bar{3}m$

Cubic

No. 222

 $P 4/n \bar{3} 2/n$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2

Origin at centre ($\bar{3}$), at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from 432Asymmetric unit $\frac{1}{4} \leq x \leq \frac{3}{4}; \frac{1}{4} \leq y \leq \frac{3}{4}; \frac{1}{4} \leq z \leq \frac{3}{4}; y \leq x; z \leq y$ Vertices $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{3}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{3}{4}, \frac{3}{4}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4}, \frac{1}{4}, z$	(3) 2 $\frac{1}{4}, y, \frac{1}{4}$	(4) 2 $x, \frac{1}{4}, \frac{1}{4}$
(5) 3^+ x, x, x	(6) 3^+ $\bar{x}, x + \frac{1}{2}, \bar{x}$	(7) 3^+ $x + \frac{1}{2}, \bar{x}, \bar{x}$	(8) 3^+ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$
(9) 3^- x, x, x	(10) 3^- $x + \frac{1}{2}, \bar{x}, \bar{x}$	(11) 3^- $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$	(12) 3^- $\bar{x}, x + \frac{1}{2}, \bar{x}$
(13) 2 $x, x, \frac{1}{4}$	(14) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$	(15) 4^- $\frac{1}{4}, \frac{1}{4}, z$	(16) 4^+ $\frac{1}{4}, \frac{1}{4}, z$
(17) 4^- $x, \frac{1}{4}, \frac{1}{4}$	(18) 2 $\frac{1}{4}, y, y$	(19) 2 $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$	(20) 4^+ $x, \frac{1}{4}, \frac{1}{4}$
(21) 4^+ $\frac{1}{4}, y, \frac{1}{4}$	(22) 2 $x, \frac{1}{4}, x$	(23) 4^- $\frac{1}{4}, y, \frac{1}{4}$	(24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$
(25) $\bar{1}$ 0,0,0	(26) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$	(27) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$	(28) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$
(29) $\bar{3}^+$ $x, x, x; 0, 0, 0$	(30) $\bar{3}^+$ $\bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{2}, 0, \frac{1}{2}$	(31) $\bar{3}^+$ $x - \frac{1}{2}, \bar{x} + 1, \bar{x}; 0, \frac{1}{2}, -\frac{1}{2}$	(32) $\bar{3}^+$ $\bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \frac{1}{2}, -\frac{1}{2}, 0$
(33) $\bar{3}^-$ $x, x, x; 0, 0, 0$	(34) $\bar{3}^-$ $x + \frac{1}{2}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{2}, \frac{1}{2}$	(35) $\bar{3}^-$ $\bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; -\frac{1}{2}, \frac{1}{2}, 0$	(36) $\bar{3}^-$ $\bar{x} + 1, x - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, -\frac{1}{2}$
(37) c x, \bar{x}, z	(38) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z	(39) 4^- $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, 0$	(40) 4^+ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$
(41) 4^- $x, -\frac{1}{4}, \frac{1}{4}; 0, -\frac{1}{4}, \frac{1}{4}$	(42) a x, y, \bar{y}	(43) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, y, y	(44) 4^+ $x, \frac{1}{4}, -\frac{1}{4}; 0, \frac{1}{4}, -\frac{1}{4}$
(45) 4^+ $-\frac{1}{4}, y, \frac{1}{4}; -\frac{1}{4}, 0, \frac{1}{4}$	(46) b \bar{x}, y, x	(47) 4^- $\frac{1}{4}, y, -\frac{1}{4}; \frac{1}{4}, 0, -\frac{1}{4}$	(48) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, y, x

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

Reflection conditions

h, k, l permutable

General:

48	i	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$OkI : k + l = 2n$
			(5) z, x, y	(6) $z, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(7) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, y$	(8) $\bar{z} + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$	$hhl : l = 2n$
			(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$	(11) $y, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(12) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$	$h00 : h = 2n$
			(13) $y, x, \bar{z} + \frac{1}{2}$	(14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(15) $y, \bar{x} + \frac{1}{2}, z$	(16) $\bar{y} + \frac{1}{2}, x, z$	
			(17) $x, z, \bar{y} + \frac{1}{2}$	(18) $\bar{x} + \frac{1}{2}, z, y$	(19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(20) $x, \bar{z} + \frac{1}{2}, y$	
			(21) $z, y, \bar{x} + \frac{1}{2}$	(22) $z, \bar{y} + \frac{1}{2}, x$	(23) $\bar{z} + \frac{1}{2}, y, x$	(24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(27) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(28) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$	(31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	(32) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$	
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$	(35) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$	(36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	
			(37) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(39) $\bar{y}, x + \frac{1}{2}, \bar{z}$	(40) $y + \frac{1}{2}, \bar{x}, \bar{z}$	
			(41) $\bar{x}, \bar{z}, y + \frac{1}{2}$	(42) $x + \frac{1}{2}, \bar{z}, \bar{y}$	(43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(44) $\bar{x}, z + \frac{1}{2}, \bar{y}$	
			(45) $\bar{z}, \bar{y}, x + \frac{1}{2}$	(46) $\bar{z}, y + \frac{1}{2}, \bar{x}$	(47) $z + \frac{1}{2}, \bar{y}, \bar{x}$	(48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	

Special: as above, plus

24	h	$..2$	$\frac{1}{4}, y, y$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, y$	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	$hkl : h + k + l = 2n$
			$y, \frac{1}{4}, y$	$y, \frac{1}{4}, \bar{y} + \frac{1}{2}$	$\bar{y} + \frac{1}{2}, \frac{1}{4}, y$	$\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y} + \frac{1}{2}$	
			$y, y, \frac{1}{4}$	$\bar{y} + \frac{1}{2}, y, \frac{1}{4}$	$y, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	
			$\frac{3}{4}, \bar{y}, \bar{y}$	$\frac{3}{4}, y + \frac{1}{2}, \bar{y}$	$\frac{3}{4}, \bar{y}, y + \frac{1}{2}$	$\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}$	
			$\bar{y}, \frac{3}{4}, \bar{y}$	$\bar{y}, \frac{3}{4}, y + \frac{1}{2}$	$y + \frac{1}{2}, \frac{3}{4}, \bar{y}$	$y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}$	
			$\bar{y}, \bar{y}, \frac{3}{4}$	$y + \frac{1}{2}, \bar{y}, \frac{3}{4}$	$\bar{y}, y + \frac{1}{2}, \frac{3}{4}$	$y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}$	

24	g	$2..$	$x, \frac{3}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, x$	$\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$
			$\frac{3}{4}, x, \frac{1}{4}$	$\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$x, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \bar{x} + \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, x$	
			$\bar{x}, \frac{1}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \bar{x}, \frac{1}{4}$	$\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \bar{x}$	$\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}$	
			$\frac{1}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$	

16	f	$.3.$	x, x, x	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$	$\bar{x} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$
			$x, x, \bar{x} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, x$	$\bar{x} + \frac{1}{2}, x, x$	
			$\bar{x}, \bar{x}, \bar{x}$	$x + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, x + \frac{1}{2}$	
			$\bar{x}, \bar{x}, x + \frac{1}{2}$	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, \bar{x}$	

12	e	$4..$	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$	$\frac{1}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$
			$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \bar{x}$	$\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}$	

12	d	$\bar{4}..$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k + l = 2n$
			$\frac{3}{4}, 0, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	

8	c	$.\bar{3}.$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h, k, l = 2n$
---	-----	-------------	-----------	-------------------------------	-------------------------------	-------------------------------	---------------------	---	---------------------	---------------------	----------------------

6	b	42.2	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
---	-----	--------	---	---	---	---	---	---	------------------------

2	a	432	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
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(Continued on page 675)

ORIGIN CHOICE 1

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[111]$ $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

ORIGIN CHOICE 2

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along $[111]$ $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}n$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (222)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

$Pm\bar{3}n$

O_h^3

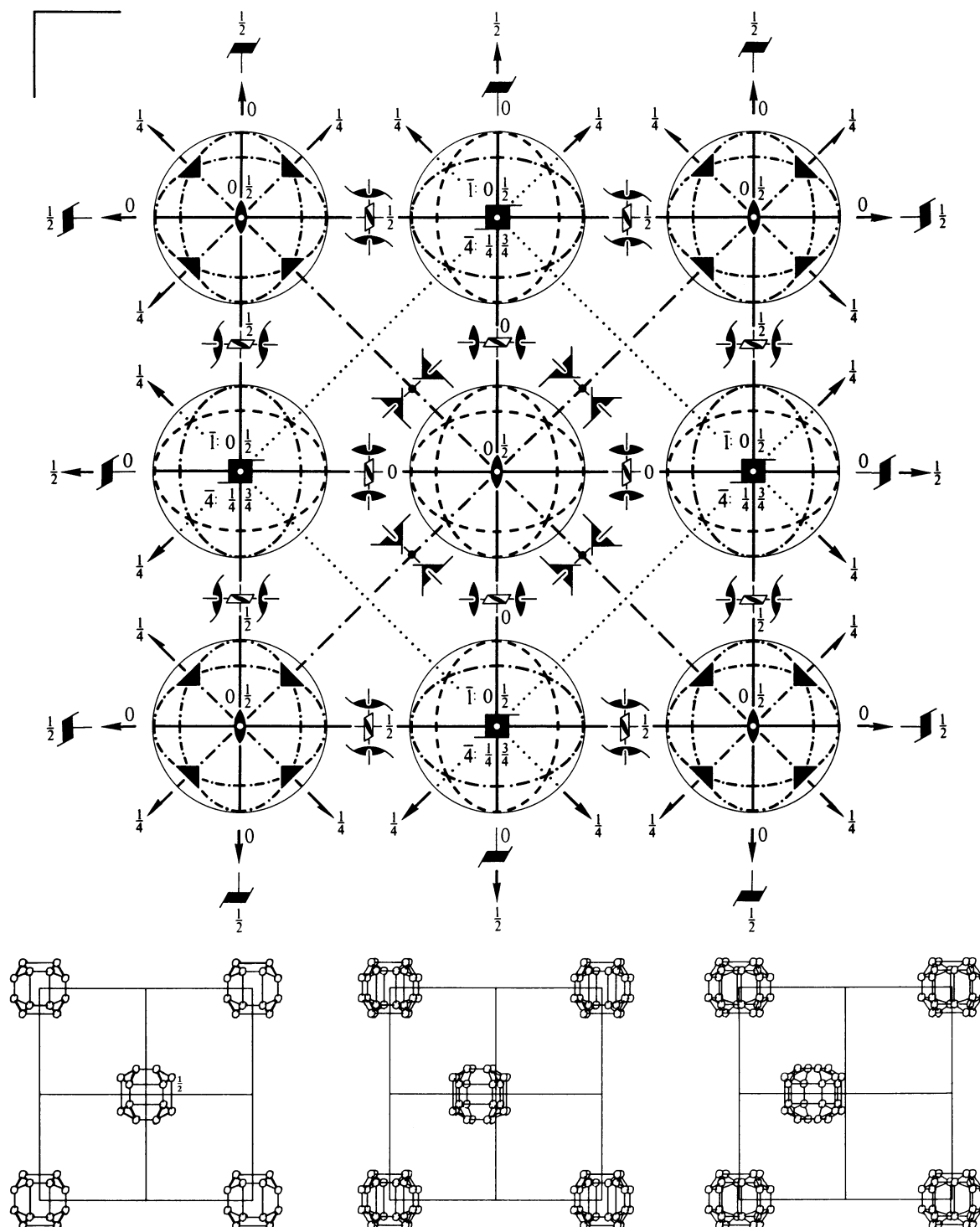
$m\bar{3}m$

Cubic

No. 223

$P 4_2/m \bar{3} 2/n$

Patterson symmetry $Pm\bar{3}m$



Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$; $z \leq \min(x, \frac{1}{2} - x, y, \frac{1}{2} - y)$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

(given on page 682)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

	Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
						h, k, l permutable General:	
48	l 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$ (26) x, y, \bar{z} (30) \bar{z}, x, y (34) y, \bar{z}, x (38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (46) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (27) x, \bar{y}, z (31) z, x, \bar{y} (35) \bar{y}, z, x (39) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (28) \bar{x}, y, z (32) z, \bar{x}, y (36) y, z, \bar{x} (40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (44) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	$hkl : l = 2n$ $h00 : h = 2n$	
						Special: as above, plus	
24	k $m..$	$0, y, z$ $z, 0, y$ $y, z, 0$ $y + \frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y}, z$ $z, 0, \bar{y}$ $\bar{y}, z, 0$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, y, \bar{z}$ $\bar{z}, 0, y$ $y, \bar{z}, 0$ $y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y}, \bar{z}$ $\bar{z}, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions	
24	j $..2$	$\frac{1}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h = 2n$	
16	i $.3.$	x, x, x \bar{x}, x, \bar{x} $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{x}$ x, \bar{x}, x $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, \bar{x}, x x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ x, x, \bar{x} \bar{x}, x, x $x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$			$hkl : h + k + l = 2n$	
12	h $mm2..$	$x, \frac{1}{2}, 0$ $\frac{1}{2}, 0, x$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$ $0, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x} + \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $0, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, x + \frac{1}{2}$	$hkl : h = 2n$	
12	g $mm2..$	$x, 0, \frac{1}{2}$ $0, \frac{1}{2}, x$ $x + \frac{1}{2}, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, x, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\frac{1}{2}, \bar{x}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $0, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h = 2n$	
12	f $mm2..$	$x, 0, 0$ $0, 0, x$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $0, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0, \bar{x}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$	
8	e $.32$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h, k, l = 2n$	
6	d $\bar{4}m.2$	$\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, \frac{1}{2}, 0$	$0, \frac{1}{4}, \frac{1}{2}$	$0, \frac{3}{4}, \frac{1}{2}$	} $hkl : h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$	
6	c $\bar{4}m.2$	$\frac{1}{4}, 0, \frac{1}{2}$	$\frac{3}{4}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{3}{4}, 0$		
6	b $mmm..$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h + k + l = 2n$
2	a $m\bar{3}.$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, \frac{1}{2}, z$

Along [111] $p6mm$
 $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I**
- | | | |
|---------------------------------------|---|--|
| [2] $P\bar{4}3n$ (218) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48 | |
| [2] $P4_232$ (208) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24 | |
| [2] $Pm\bar{3}1$ ($Pm\bar{3}$, 200) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36 | |
| { | [3] $P4_2/m12/n(P4_2/mmc, 131)$ | 1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40 |
| | [3] $P4_2/m12/n(P4_2/mmc, 131)$ | 1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44 |
| | [3] $P4_2/m12/n(P4_2/mmc, 131)$ | 1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48 |
| { | [4] $P1\bar{3}2/n(R\bar{3}c, 167)$ | 1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48 |
| | [4] $P1\bar{3}2/n(R\bar{3}c, 167)$ | 1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48 |
| | [4] $P1\bar{3}2/n(R\bar{3}c, 167)$ | 1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46 |
| | [4] $P1\bar{3}2/n(R\bar{3}c, 167)$ | 1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46 |

IIa none

IIb [4] $Ia\bar{3}d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (230)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pm\bar{3}n$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (223)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x}, x, \bar{x}$ | (7) $3^+ x, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- x, \bar{x}, \bar{x}$ | (11) $3^- \bar{x}, \bar{x}, x$ | (12) $3^- \bar{x}, x, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (14) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ | (15) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ | (16) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0)$ $x, \frac{1}{2}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, y$ | (19) 2 $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0)$ $\frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, x$ | (23) $4^-(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ |
| (25) $\bar{1}$ $0, 0, 0$ | (26) m $x, y, 0$ | (27) m $x, 0, z$ | (28) m $0, y, z$ |
| (29) $\bar{3}^+ x, x, x; 0, 0, 0$ | (30) $\bar{3}^+ \bar{x}, x, \bar{x}; 0, 0, 0$ | (31) $\bar{3}^+ x, \bar{x}, \bar{x}; 0, 0, 0$ | (32) $\bar{3}^+ \bar{x}, \bar{x}, x; 0, 0, 0$ |
| (33) $\bar{3}^- x, x, x; 0, 0, 0$ | (34) $\bar{3}^- x, \bar{x}, \bar{x}; 0, 0, 0$ | (35) $\bar{3}^- \bar{x}, \bar{x}, x; 0, 0, 0$ | (36) $\bar{3}^- \bar{x}, x, \bar{x}; 0, 0, 0$ |
| (37) c $x + \frac{1}{2}, \bar{x}, z$ | (38) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z | (39) $\bar{4}^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ | (40) $\bar{4}^+ \frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ |
| (41) $\bar{4}^- x, 0, \frac{1}{2}; \frac{1}{4}, 0, \frac{1}{2}$ | (42) a $x, y + \frac{1}{2}, \bar{y}$ | (43) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, y, y | (44) $\bar{4}^+ x, \frac{1}{2}, 0; \frac{1}{4}, \frac{1}{2}, 0$ |
| (45) $\bar{4}^+ 0, y, \frac{1}{2}; 0, \frac{1}{4}, \frac{1}{2}$ | (46) b $\bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, 0; \frac{1}{2}, \frac{1}{4}, 0$ | (48) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, y, x |

$Pn\bar{3}m$

O_h^4

$m\bar{3}m$

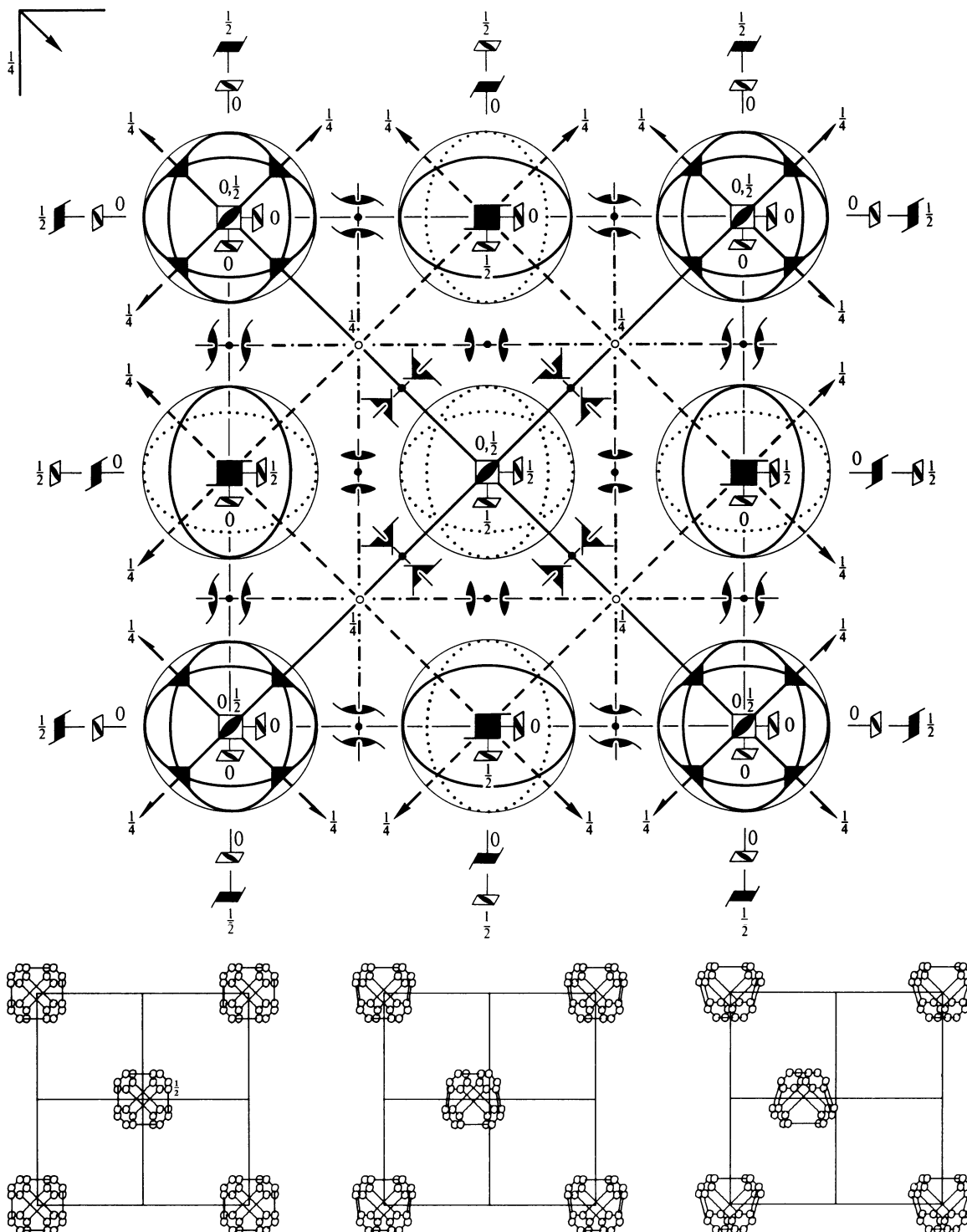
Cubic

No. 224

$P 4_2/n \bar{3} 2/m$

Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1



Origin at $\bar{4}3m$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq x; \max(x - \frac{1}{2}, -y) \leq z \leq \min(\frac{1}{2} - x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

(given on page 683)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

	Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions					
48	l 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{x}, y, \bar{z} (4) x, \bar{y}, \bar{z} (5) z, x, y (6) z, \bar{x}, \bar{y} (7) \bar{z}, \bar{x}, y (8) \bar{z}, x, \bar{y} (9) y, z, x (10) \bar{y}, z, \bar{x} (11) y, \bar{z}, \bar{x} (12) \bar{y}, \bar{z}, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (25) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (26) $x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (27) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (28) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (29) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (30) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}$ (31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (32) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (33) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (34) $y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (35) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (37) \bar{y}, \bar{x}, z (38) y, x, z (39) \bar{y}, x, \bar{z} (40) y, \bar{x}, \bar{z} (41) \bar{x}, \bar{z}, y (42) x, \bar{z}, \bar{y} (43) x, z, y (44) \bar{x}, z, \bar{y} (45) \bar{z}, \bar{y}, x (46) \bar{z}, y, \bar{x} (47) z, \bar{y}, \bar{x} (48) z, y, x	$Ok\bar{l} : k + l = 2n$ $h00 : h = 2n$					
			Special: as above, plus					
24	k $\dots m$	x, x, z z, x, x x, z, x $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $z + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, \bar{x}, z z, \bar{x}, \bar{x} \bar{x}, z, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	\bar{x}, x, \bar{z} \bar{z}, \bar{x}, x x, \bar{z}, \bar{x} $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	x, \bar{x}, \bar{z} \bar{z}, x, \bar{x} \bar{x}, \bar{z}, x $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	no extra conditions		
24	j $\dots 2$	$\frac{1}{4}, y, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, \bar{y}$ $y, \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\frac{3}{4}, y + \frac{1}{2}, \bar{y}$ $y, \frac{1}{4}, y + \frac{1}{2}$	$\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $y, y + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{y}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{1}{2}, y$ $y + \frac{1}{2}, \bar{y}, \frac{3}{4}$	$y + \frac{1}{2}, \frac{1}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\bar{y}, \frac{1}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, y, \frac{3}{4}$	$y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\bar{y}, \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, y, \frac{1}{4}$	no extra conditions
24	i $\dots 2$	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, y$ $\bar{y}, \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\frac{3}{4}, y + \frac{1}{2}, y$ $\bar{y}, \frac{1}{4}, y + \frac{1}{2}$	$\frac{3}{4}, y, y + \frac{1}{2}$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, \bar{y}$ $\bar{y} + \frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$ $y + \frac{1}{2}, \bar{y}, \frac{3}{4}$	$\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$ $y, \frac{1}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y}, \frac{3}{4}$	$\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$ $y, \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, \bar{y}, \frac{1}{4}$	no extra conditions
24	h $2 \dots$	$x, 0, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$ $0, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$ $0, x, \frac{1}{2}$	$\frac{1}{2}, x, 0$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $0, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $0, x + \frac{1}{2}, \frac{1}{2}$ $x, \frac{1}{2}, 0$	$0, \frac{1}{2}, x$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, 0, x$	$0, \frac{1}{2}, \bar{x}$ $0, \frac{1}{2}, x + \frac{1}{2}$ $\frac{1}{2}, 0, x + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x}$	$hkl : h + k + l = 2n$
12	g $2 \dots mm$	$x, 0, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0, x, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, x$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0, 0, \bar{x}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
12	f $2 \dots 22$	$\frac{1}{4}, 0, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, 0, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{4}, 0$ $0, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{2}, \frac{3}{4}, 0$ $0, \frac{3}{4}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k + l = 2n$
8	e $\dots 3m$	x, x, x $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, \bar{x}, x $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, x, \bar{x} $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions	no extra conditions	
6	d $\bar{4}2 \dots m$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : h + k + l = 2n$	$hkl : h + k + l = 2n$	
4	c $\dots \bar{3}m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$	$hkl : h + k, h + l, k + l = 2n$	
4	b $\dots \bar{3}m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$	$hkl : h + k, h + l, k + l = 2n$	
2	a $\bar{4}3m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$	$hkl : h + k + l = 2n$	

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [111] $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at x, x, $\frac{1}{4}$

(Continued on page 683)

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4_2/n12/m(P4_2/nnm, 134)$	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4_2/n12/m(P4_2/nnm, 134)$	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4_2/n12/m(P4_2/nnm, 134)$	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb [2] $Fd\bar{3}c$ ($a' = 2a, b' = 2b, c' = 2c$) (228); [2] $Fd\bar{3}m$ ($a' = 2a, b' = 2b, c' = 2c$) (227)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}m$ ($a' = 3a, b' = 3b, c' = 3c$) (224)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

ORIGIN CHOICE 1

Symmetry operations

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) $3^+ x,x,x$	(6) $3^+ \bar{x},x,\bar{x}$	(7) $3^+ x,\bar{x},\bar{x}$	(8) $3^+ \bar{x},\bar{x},x$
(9) $3^- x,x,x$	(10) $3^- x,\bar{x},\bar{x}$	(11) $3^- \bar{x},\bar{x},x$	(12) $3^- \bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0) x,x,\frac{1}{4}$	(14) $2 x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2}) \frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2}) 0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0) x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4},y,y$	(19) $2 \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0) x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0) \frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2}) x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0) 0,y,\frac{1}{2}$	(24) $2 \bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1} \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(26) $n(\frac{1}{2},\frac{1}{2},0) x,y,\frac{1}{4}$	(27) $n(\frac{1}{2},0,\frac{1}{2}) x,\frac{1}{4},z$	(28) $n(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4},y,z$
(29) $3^+ x,x,x; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(30) $3^+ \bar{x}-1,x+1,\bar{x}; -\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(31) $3^+ x,\bar{x}+1,\bar{x}; \frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(32) $3^+ \bar{x}+1,\bar{x},x; \frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $3^- x,x,x; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(34) $3^- x+1,\bar{x}-1,\bar{x}; \frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(35) $3^- \bar{x},\bar{x}+1,x; -\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(36) $3^- \bar{x}+1,x,\bar{x}; \frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) $m x,\bar{x},z$	(38) $m x,x,z$	(39) $\bar{4}^- 0,0,z; 0,0,0$	(40) $\bar{4}^+ 0,0,z; 0,0,0$
(41) $\bar{4}^- x,0,0; 0,0,0$	(42) $m x,y,\bar{y}$	(43) $m x,y,y$	(44) $\bar{4}^+ x,0,0; 0,0,0$
(45) $\bar{4}^+ 0,y,0; 0,0,0$	(46) $m \bar{x},y,x$	(47) $\bar{4}^- 0,y,0; 0,0,0$	(48) $m x,y,x$

ORIGIN CHOICE 2

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+ x,x,x$	(6) $3^+ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^+ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^+ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^- x,x,x$	(10) $3^- x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^- \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^- \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0) x,x,0$	(14) 2 $x,\bar{x},0$	(15) $4^-(0,0,\frac{1}{2}) \frac{1}{4},-\frac{1}{4},z$	(16) $4^+(0,0,\frac{1}{2}) -\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{2},0,0) x,\frac{1}{4},-\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2}) 0,y,y$	(19) 2 $0,y,\bar{y}$	(20) $4^+(\frac{1}{2},0,0) x,-\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{2},0) \frac{1}{4},y,-\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2}) x,0,x$	(23) $4^-(0,\frac{1}{2},0) -\frac{1}{4},y,\frac{1}{4}$	(24) 2 $\bar{x},0,x$
(25) $\bar{1} 0,0,0$	(26) $n(\frac{1}{2},\frac{1}{2},0) x,y,0$	(27) $n(\frac{1}{2},0,\frac{1}{2}) x,0,z$	(28) $n(0,\frac{1}{2},\frac{1}{2}) 0,y,z$
(29) $3^+ x,x,x; 0,0,0$	(30) $3^+ \bar{x}-1,x+\frac{1}{2},\bar{x}; -\frac{1}{2},0,\frac{1}{2}$	(31) $3^+ x-\frac{1}{2},\bar{x}+1,\bar{x}; 0,\frac{1}{2},-\frac{1}{2}$	(32) $3^+ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x; \frac{1}{2},-\frac{1}{2},0$
(33) $3^- x,x,x; 0,0,0$	(34) $3^- x+\frac{1}{2},\bar{x}-1,\bar{x}; 0,-\frac{1}{2},\frac{1}{2}$	(35) $3^- \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x; -\frac{1}{2},\frac{1}{2},0$	(36) $3^- \bar{x}+1,x-\frac{1}{2},\bar{x}; \frac{1}{2},0,-\frac{1}{2}$
(37) $m x+\frac{1}{2},\bar{x},z$	(38) $m x,x,z$	(39) $\bar{4}^- \frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(40) $\bar{4}^+ \frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^- x,\frac{1}{4},\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(42) $m x,y+\frac{1}{2},\bar{y}$	(43) $m x,y,y$	(44) $\bar{4}^+ x,\frac{1}{4},\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+ \frac{1}{4},y,\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(46) $m \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^- \frac{1}{4},y,\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(48) $m x,y,x$

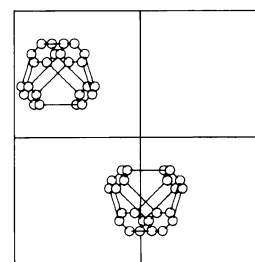
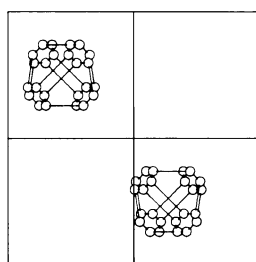
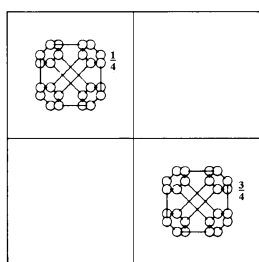
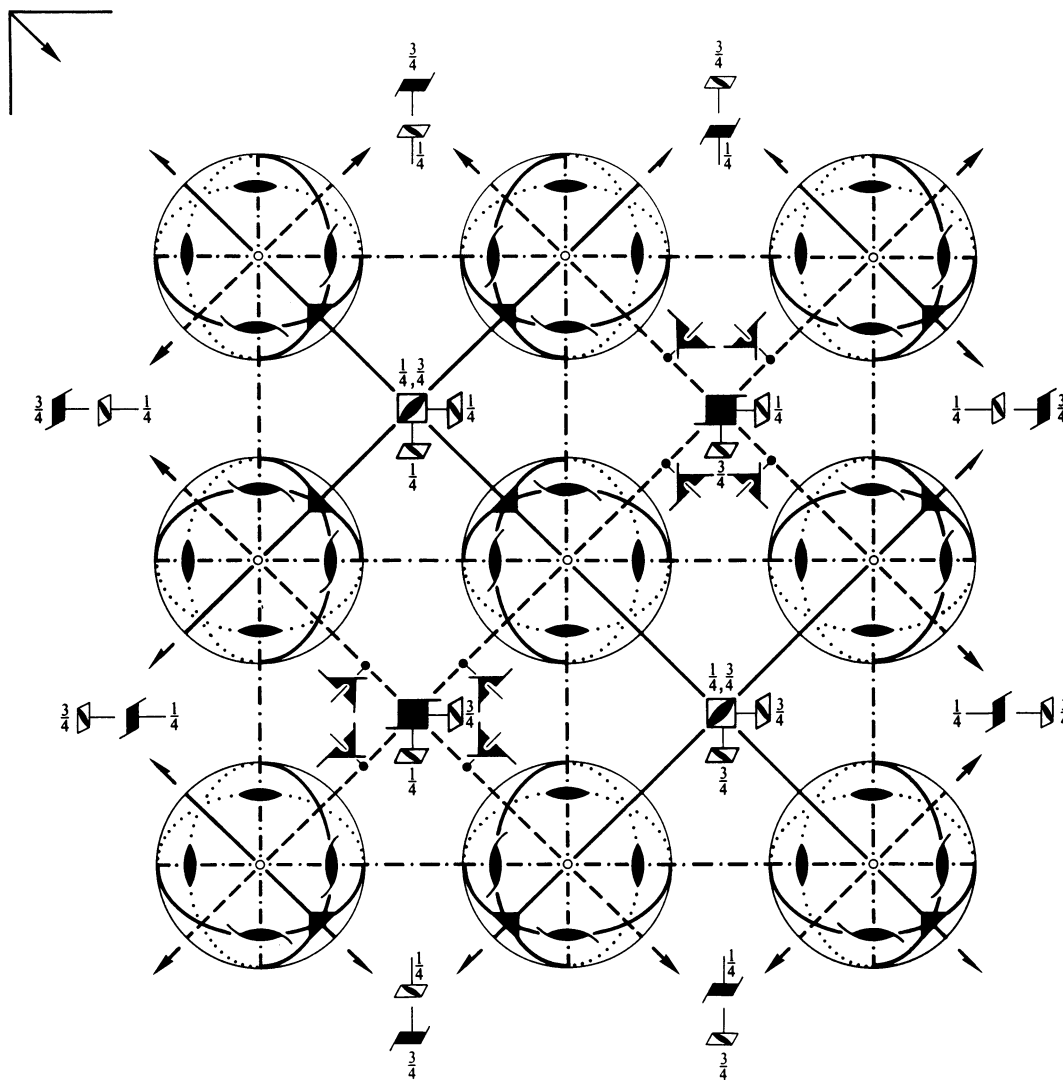
$Pn\bar{3}m$ O_h^4 $m\bar{3}m$

Cubic

No. 224

 $P 4_2/n \bar{3} 2/m$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2



Origin at centre ($\bar{3}m$), at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{4}3m$

Asymmetric unit $\frac{1}{4} \leq x \leq \frac{3}{4}; \frac{1}{4} \leq y \leq \frac{3}{4}; 0 \leq z \leq \frac{1}{2}; y \leq x; \max(x - \frac{1}{2}, \frac{1}{2} - y) \leq z \leq \min(y, 1 - x)$

Vertices $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{3}{4}, \frac{1}{4} \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \quad \frac{1}{2}, \frac{1}{2}, 0$

Symmetry operations

(given on page 683)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
					h, k, l permutable General:	
48 l 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (41) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ (45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $z, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (10) $\bar{y} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$ (14) $\bar{y}, \bar{x}, \bar{z}$ (18) $\bar{x}, z + \frac{1}{2}, y + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$ (26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (30) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$ (34) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (38) y, x, z (42) $x, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (46) $\bar{z} + \frac{1}{2}, y, \bar{x} + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, y$ (11) $y, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (15) $y + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ (19) $\bar{x}, \bar{z}, \bar{y}$ (23) $\bar{z}, y + \frac{1}{2}, x + \frac{1}{2}$ (27) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$ (35) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$ (39) $\bar{y} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$ (43) x, z, y (47) $z, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{z} + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$ (16) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$ (24) $\bar{z}, \bar{y}, \bar{x}$ (28) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (32) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ (40) $y, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (44) $\bar{x} + \frac{1}{2}, z, \bar{y} + \frac{1}{2}$ (48) z, y, x	$Ok l : k + l = 2n$ $h00 : h = 2n$	
24 k $\dots m$	x, x, z z, x, x x, z, x $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ $z + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $z, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{z}$ $\bar{x}, z + \frac{1}{2}, x + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ $x, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ $\bar{x}, \bar{z}, \bar{x}$ $\bar{z}, x + \frac{1}{2}, x + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$ $\bar{x}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ $\bar{z}, \bar{x}, \bar{x}$	Special: as above, plus no extra conditions	
24 j $\dots 2$	$\frac{1}{2}, y, \bar{y}$ $\bar{y}, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$ $\frac{1}{2}, \bar{y}, y$ $y, \frac{1}{2}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$0, \bar{y} + \frac{1}{2}, \bar{y}$ $\bar{y}, 0, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y}, 0$ $0, y + \frac{1}{2}, y$ $y, 0, y + \frac{1}{2}$ $y + \frac{1}{2}, y, 0$	$0, y, y + \frac{1}{2}$ $y + \frac{1}{2}, 0, y$ $y, y + \frac{1}{2}, 0$ $0, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, 0, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, 0$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, y + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}$ $y + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions	
24 i $\dots 2$	$\frac{1}{2}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{2}, y$ $y, y + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y} + \frac{1}{2}, y + \frac{1}{2}$ $y + \frac{1}{2}, 0, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, y + \frac{1}{2}, 0$ $0, y + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, 0, y + \frac{1}{2}$ $y + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	$0, y, \bar{y}$ $\bar{y}, 0, y$ $y, \bar{y}, 0$ $0, \bar{y}, y$ $y, 0, \bar{y}$ $\bar{y}, y, 0$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{y}$ $\bar{y}, \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y}, \frac{1}{2}$ $\frac{1}{2}, y + \frac{1}{2}, y$ $y, \frac{1}{2}, y + \frac{1}{2}$ $y + \frac{1}{2}, y, \frac{1}{2}$	no extra conditions	
24 h $2 \dots$	$x, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$	$\frac{3}{4}, x, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$ $x, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, x$ $\frac{1}{4}, \frac{3}{4}, \bar{x}$ $\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{3}{4}, \frac{1}{4}, x$	$hkl : h + k + l = 2n$
12 g $2 \dots mm$	$x, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$	$hkl : h + k + l = 2n$
12 f $2 \dots 22$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$0, \frac{1}{4}, \frac{3}{4}$ $0, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, 0, \frac{1}{4}$ $\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h + k + l = 2n$
8 e $\dots 3m$	x, x, x $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ $\bar{x}, \bar{x}, \bar{x}$	$\bar{x} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions	
6 d $\bar{4}2 \dots m$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
4 c $\dots \bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$		$hkl : h + k, h + l, k + l = 2n$
4 b $\dots \bar{3}m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$		$hkl : h + k, h + l, k + l = 2n$
2 a $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$				$hkl : h + k + l = 2n$

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{4}, \frac{1}{4}, z$

(Continued on page 683)

Along [111] $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4_2/n12/m(P4_2/nnm, 134)$	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4_2/n12/m(P4_2/nnm, 134)$	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4_2/n12/m(P4_2/nnm, 134)$	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/m(R\bar{3}m, 166)$	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb [2] $Fd\bar{3}c$ ($a' = 2a, b' = 2b, c' = 2c$) (228); [2] $Fd\bar{3}m$ ($a' = 2a, b' = 2b, c' = 2c$) (227)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}m$ ($a' = 3a, b' = 3b, c' = 3c$) (224)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

ORIGIN CHOICE 1

Symmetry operations

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) $3^+ x,x,x$	(6) $3^+ \bar{x},x,\bar{x}$	(7) $3^+ x,\bar{x},\bar{x}$	(8) $3^+ \bar{x},\bar{x},x$
(9) $3^- x,x,x$	(10) $3^- x,\bar{x},\bar{x}$	(11) $3^- \bar{x},\bar{x},x$	(12) $3^- \bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0) x,x,\frac{1}{4}$	(14) $2 x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2}) \frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2}) 0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0) x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4},y,y$	(19) $2 \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0) x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0) \frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2}) x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0) 0,y,\frac{1}{2}$	(24) $2 \bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1} \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(26) $n(\frac{1}{2},\frac{1}{2},0) x,y,\frac{1}{4}$	(27) $n(\frac{1}{2},0,\frac{1}{2}) x,\frac{1}{4},z$	(28) $n(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4},y,z$
(29) $3^+ x,x,x; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(30) $3^+ \bar{x}-1,x+1,\bar{x}; -\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(31) $3^+ x,\bar{x}+1,\bar{x}; \frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(32) $3^+ \bar{x}+1,\bar{x},x; \frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $3^- x,x,x; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(34) $3^- x+1,\bar{x}-1,\bar{x}; \frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(35) $3^- \bar{x},\bar{x}+1,x; -\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(36) $3^- \bar{x}+1,x,\bar{x}; \frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) $m x,\bar{x},z$	(38) $m x,x,z$	(39) $\bar{4}^- 0,0,z; 0,0,0$	(40) $\bar{4}^+ 0,0,z; 0,0,0$
(41) $\bar{4}^- x,0,0; 0,0,0$	(42) $m x,y,\bar{y}$	(43) $m x,y,y$	(44) $\bar{4}^+ x,0,0; 0,0,0$
(45) $\bar{4}^+ 0,y,0; 0,0,0$	(46) $m \bar{x},y,x$	(47) $\bar{4}^- 0,y,0; 0,0,0$	(48) $m x,y,x$

ORIGIN CHOICE 2

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+ x,x,x$	(6) $3^+ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^+ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^+ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^- x,x,x$	(10) $3^- x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^- \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^- \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0) x,x,0$	(14) 2 $x,\bar{x},0$	(15) $4^-(0,0,\frac{1}{2}) \frac{1}{4},-\frac{1}{4},z$	(16) $4^+(0,0,\frac{1}{2}) -\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{2},0,0) x,\frac{1}{4},-\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2}) 0,y,y$	(19) 2 $0,y,\bar{y}$	(20) $4^+(\frac{1}{2},0,0) x,-\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{2},0) \frac{1}{4},y,-\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2}) x,0,x$	(23) $4^-(0,\frac{1}{2},0) -\frac{1}{4},y,\frac{1}{4}$	(24) 2 $\bar{x},0,x$
(25) $\bar{1} 0,0,0$	(26) $n(\frac{1}{2},\frac{1}{2},0) x,y,0$	(27) $n(\frac{1}{2},0,\frac{1}{2}) x,0,z$	(28) $n(0,\frac{1}{2},\frac{1}{2}) 0,y,z$
(29) $3^+ x,x,x; 0,0,0$	(30) $3^+ \bar{x}-1,x+\frac{1}{2},\bar{x}; -\frac{1}{2},0,\frac{1}{2}$	(31) $3^+ x-\frac{1}{2},\bar{x}+1,\bar{x}; 0,\frac{1}{2},-\frac{1}{2}$	(32) $3^+ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x; \frac{1}{2},-\frac{1}{2},0$
(33) $3^- x,x,x; 0,0,0$	(34) $3^- x+\frac{1}{2},\bar{x}-1,\bar{x}; 0,-\frac{1}{2},\frac{1}{2}$	(35) $3^- \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x; -\frac{1}{2},\frac{1}{2},0$	(36) $3^- \bar{x}+1,x-\frac{1}{2},\bar{x}; \frac{1}{2},0,-\frac{1}{2}$
(37) $m x+\frac{1}{2},\bar{x},z$	(38) $m x,x,z$	(39) $\bar{4}^- \frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(40) $\bar{4}^+ \frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^- x,\frac{1}{4},\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(42) $m x,y+\frac{1}{2},\bar{y}$	(43) $m x,y,y$	(44) $\bar{4}^+ x,\frac{1}{4},\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+ \frac{1}{4},y,\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(46) $m \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^- \frac{1}{4},y,\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(48) $m x,y,x$

$Fm\bar{3}m$

O_h^5

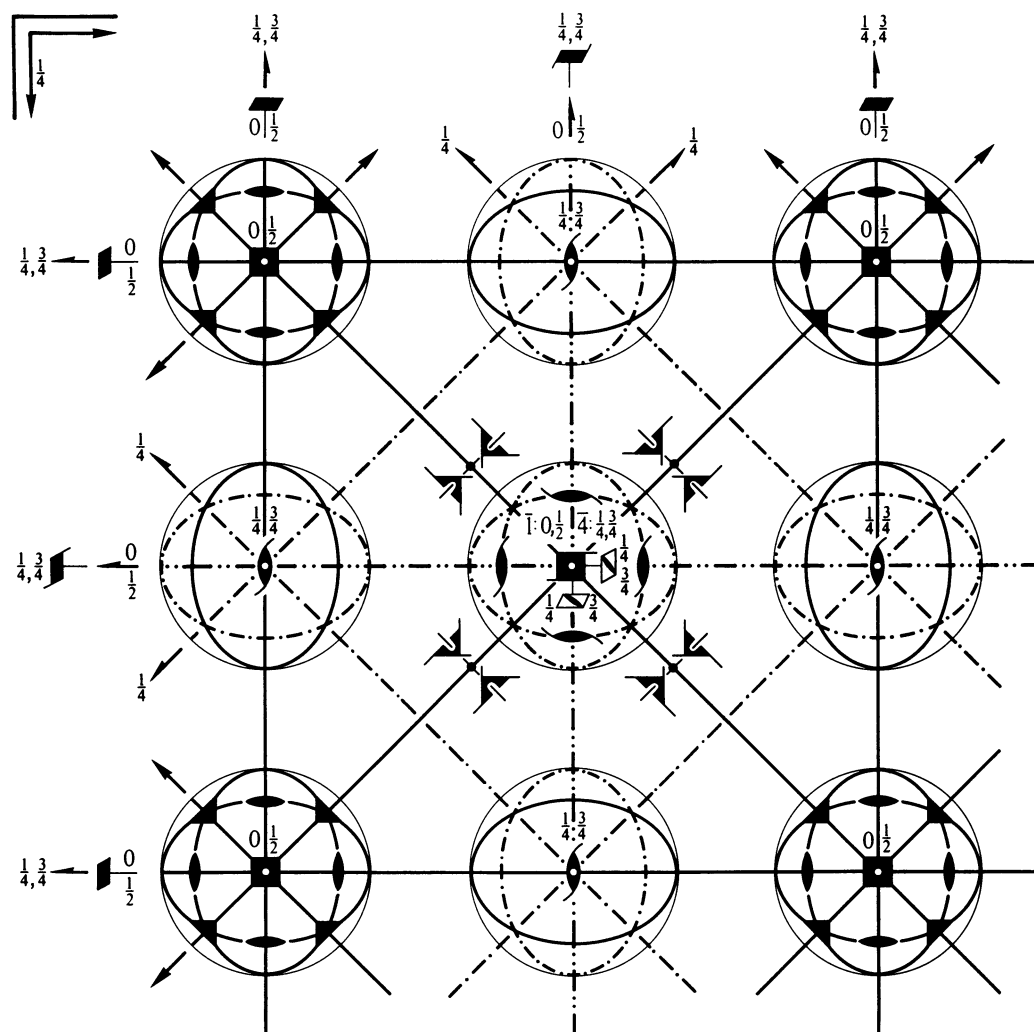
$m\bar{3}m$

Cubic

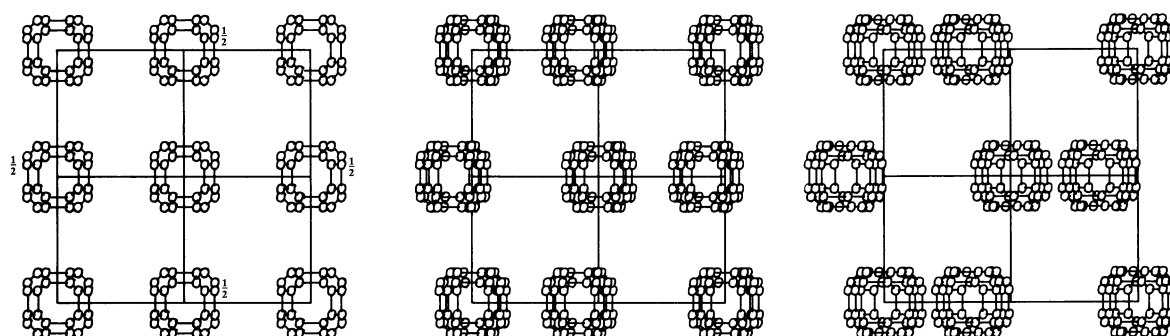
No. 225

$F 4/m \bar{3} 2/m$

Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at centre ($m\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq \frac{1}{4}$; $y \leq \min(x, \frac{1}{2} - x)$; $z \leq y$

Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

(given on page 691)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$				h, k, l permutable General:
192 l 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) y, x, \bar{z} (17) x, z, \bar{y} (21) z, y, \bar{x} (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) \bar{y}, \bar{x}, z (41) \bar{x}, \bar{z}, y (45) \bar{z}, \bar{y}, x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y}, \bar{x}, \bar{z}$ (18) \bar{x}, z, y (22) z, \bar{y}, x (26) x, y, \bar{z} (30) \bar{z}, x, y (34) y, \bar{z}, x (38) y, x, z (42) x, \bar{z}, \bar{y} (46) \bar{z}, y, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, z (19) $\bar{x}, \bar{z}, \bar{y}$ (23) \bar{z}, y, x (27) x, \bar{y}, z (31) z, x, \bar{y} (35) \bar{y}, z, x (39) \bar{y}, x, \bar{z} (43) x, z, y (47) z, \bar{y}, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, z (20) x, \bar{z}, y (24) $\bar{z}, \bar{y}, \bar{x}$ (28) \bar{x}, y, z (32) z, \bar{x}, y (36) y, z, \bar{x} (40) y, \bar{x}, \bar{z} (44) \bar{x}, z, \bar{y} (48) z, y, x	$hkl : h+k, h+l, k+l = 2n$ $OkI : k, l = 2n$ $hhl : h+l = 2n$ $h00 : h = 2n$			
96 k $\dots m$	x, x, z \bar{z}, \bar{x}, x x, x, \bar{z} $\bar{x}, \bar{z}, \bar{x}$	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x} $\bar{x}, \bar{x}, \bar{z}$ x, \bar{z}, x	\bar{x}, x, \bar{z} x, z, x x, \bar{x}, z z, x, \bar{x}	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x} \bar{x}, x, z z, \bar{x}, x	z, x, x x, \bar{z}, \bar{x} x, z, \bar{x} \bar{z}, x, x	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x \bar{x}, z, x $\bar{z}, \bar{x}, \bar{x}$	no extra conditions	
96 j $m \dots$	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions	
48 i $m \dots m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	no extra conditions	
48 h $m \dots m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions	
48 g $2 \dots mm$	$x, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\bar{x}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{1}{4}, \bar{x}$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x$	$hkl : h = 2n$	
32 f $\dots 3m$	x, x, x x, x, \bar{x}	\bar{x}, \bar{x}, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x			no extra conditions	
24 e $4m \dots m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions	
24 d $m \dots mm$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h = 2n$	
8 c $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$					$hkl : h = 2n$	
4 b $m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						no extra conditions	
4 a $m\bar{3}m$	$0, 0, 0$						no extra conditions	

Symmetry of special projections

Along $[001]$ $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $0, 0, z$

Along $[111]$ $p6mm$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along $[110]$ $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+	
	[2] $F432$ (209)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+	
	[2] $Fm\bar{3}1$ ($Fm\bar{3}$, 202)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+	
	{	[3] $F4/m12/m(I4/mmm, 139)$	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
		[3] $F4/m12/m(I4/mmm, 139)$	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
		[3] $F4/m12/m(I4/mmm, 139)$	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	{	[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
		[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
		[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
		[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	{	[4] $Pn\bar{3}m$ (224)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2}, \frac{1}{2}, 0)$
		[4] $Pn\bar{3}m$ (224)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2}, \frac{1}{2}, 0)$
		[4] $Pn\bar{3}m$ (224)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2}, \frac{1}{2}, 0)$
		[4] $Pn\bar{3}m$ (224)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2}, \frac{1}{2}, 0)$
		[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
		[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0, \frac{1}{2}, \frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$
		[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2}, \frac{1}{2}, 0)$
[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0, \frac{1}{2}, \frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2}, \frac{1}{2}, 0)$		

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fm\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (225)

Minimal non-isomorphic supergroups

I none

II [2] $Pm\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (221)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|-------------------------------|---|---|--|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) 2 x,x,0 | (14) 2 x, $\bar{x},0$ | (15) 4 ⁻ 0,0,z | (16) 4 ⁺ 0,0,z |
| (17) 4 ⁻ x,0,0 | (18) 2 0,y,y | (19) 2 0,y, \bar{y} | (20) 4 ⁺ x,0,0 |
| (21) 4 ⁺ 0,y,0 | (22) 2 x,0,x | (23) 4 ⁻ 0,y,0 | (24) 2 $\bar{x},0,x$ |
| (25) $\bar{1}$ 0,0,0 | (26) m x,y,0 | (27) m x,0,z | (28) m 0,y,z |
| (29) $\bar{3}^+$ x,x,x; 0,0,0 | (30) $\bar{3}^+$ \bar{x},x,\bar{x} ; 0,0,0 | (31) $\bar{3}^+$ x, \bar{x},\bar{x} ; 0,0,0 | (32) $\bar{3}^+$ \bar{x},\bar{x},x ; 0,0,0 |
| (33) $\bar{3}^-$ x,x,x; 0,0,0 | (34) $\bar{3}^-$ x, \bar{x},\bar{x} ; 0,0,0 | (35) $\bar{3}^-$ \bar{x},\bar{x},x ; 0,0,0 | (36) $\bar{3}^-$ \bar{x},x,\bar{x} ; 0,0,0 |
| (37) m x, \bar{x},z | (38) m x,x,z | (39) $\bar{4}^-$ 0,0,z; 0,0,0 | (40) $\bar{4}^+$ 0,0,z; 0,0,0 |
| (41) $\bar{4}^-$ x,0,0; 0,0,0 | (42) m x,y, \bar{y} | (43) m x,y,y | (44) $\bar{4}^+$ x,0,0; 0,0,0 |
| (45) $\bar{4}^+$ 0,y,0; 0,0,0 | (46) m \bar{x},y,x | (47) $\bar{4}^-$ 0,y,0; 0,0,0 | (48) m x,y,x |

For (0, $\frac{1}{2},\frac{1}{2}$)+ set

- | | | | |
|---|---|--|--|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) 0, $\frac{1}{4},z$ | (3) 2(0, $\frac{1}{2},0$) 0,y, $\frac{1}{4}$ | (4) 2 x, $\frac{1}{4},\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $-\frac{1}{3},x-\frac{1}{6},x$ | (6) 3 ⁺ $\bar{x},x+\frac{1}{2},\bar{x}$ | (7) 3 ⁺ ($-\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) 3 ⁺ $\bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $-\frac{1}{6},x+\frac{1}{6},x$ | (10) 3 ⁻ ($-\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) 3 ⁻ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ | (12) 3 ⁻ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ |
| (13) 2($\frac{1}{4},\frac{1}{4},0$) x,x $+\frac{1}{4},\frac{1}{4}$ | (14) 2($-\frac{1}{4},\frac{1}{4},0$) x, $\bar{x}+\frac{1}{4},\frac{1}{4}$ | (15) 4 ⁻ (0,0, $\frac{1}{2}$) $\frac{1}{4},\frac{1}{4},z$ | (16) 4 ⁺ (0,0, $\frac{1}{2}$) $-\frac{1}{4},\frac{1}{4},z$ |
| (17) 4 ⁻ x, $\frac{1}{2},0$ | (18) 2(0, $\frac{1}{2},\frac{1}{2}$) 0,y,y | (19) 2 0,y $+\frac{1}{2},\bar{y}$ | (20) 4 ⁺ x,0, $\frac{1}{2}$ |
| (21) 4 ⁺ (0, $\frac{1}{2},0$) $\frac{1}{4},y,\frac{1}{4}$ | (22) 2($\frac{1}{4},0,\frac{1}{4}$) x $-\frac{1}{4},\frac{1}{4},x$ | (23) 4 ⁻ (0, $\frac{1}{2},0$) $-\frac{1}{4},y,\frac{1}{4}$ | (24) 2($-\frac{1}{4},0,\frac{1}{4}$) $\bar{x}+\frac{1}{4},\frac{1}{4},x$ |
| (25) $\bar{1}$ 0, $\frac{1}{4},\frac{1}{4}$ | (26) b x,y, $\frac{1}{4}$ | (27) c x, $\frac{1}{4},z$ | (28) n(0, $\frac{1}{2},\frac{1}{2}$) 0,y,z |
| (29) $\bar{3}^+$ x,x $+\frac{1}{2},x$; 0, $\frac{1}{2},0$ | (30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{1}{2},0,\frac{1}{2}$ | (31) $\bar{3}^+$ x, $\bar{x}+\frac{1}{2},\bar{x}$; 0, $\frac{1}{2},0$ | (32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{1}{2},0,\frac{1}{2}$ |
| (33) $\bar{3}^-$ x $-\frac{1}{2},x-\frac{1}{2},x$; 0,0, $\frac{1}{2}$ | (34) $\bar{3}^-$ x $+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; 0,0, $\frac{1}{2}$ | (35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{1}{2},\frac{1}{2},0$ | (36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$ |
| (37) g($-\frac{1}{4},\frac{1}{4},\frac{1}{2}$) x $+\frac{1}{4},\bar{x},z$ | (38) g($\frac{1}{4},\frac{1}{4},\frac{1}{2}$) x $-\frac{1}{4},x,z$ | (39) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |
| (41) $\bar{4}^-$ x,0, $\frac{1}{2}$; 0,0, $\frac{1}{2}$ | (42) m x,y $+\frac{1}{2},\bar{y}$ | (43) g(0, $\frac{1}{2},\frac{1}{2}$) x,y,y | (44) $\bar{4}^+$ x, $\frac{1}{2},0$; 0, $\frac{1}{2},0$ |
| (45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (46) g($-\frac{1}{4},\frac{1}{2},\frac{1}{4}$) $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (48) g($\frac{1}{4},\frac{1}{2},\frac{1}{4}$) x $-\frac{1}{4},y,x$ |

For ($\frac{1}{2},0,\frac{1}{2}$)+ set

- | | | | |
|---|---|---|--|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4},0,z$ | (3) 2 $\frac{1}{4},y,\frac{1}{4}$ | (4) 2($\frac{1}{2},0,0$) x,0, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $+\frac{1}{6},x-\frac{1}{6},x$ | (6) 3 ⁺ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ | (7) 3 ⁺ x $+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) 3 ⁺ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ |
| (9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $-\frac{1}{6},x-\frac{1}{6},x$ | (10) 3 ⁻ x $+\frac{1}{2},\bar{x},\bar{x}$ | (11) 3 ⁻ $\bar{x}+\frac{1}{2},\bar{x},x$ | (12) 3 ⁻ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}-\frac{1}{6},x+\frac{1}{6},\bar{x}$ |
| (13) 2($\frac{1}{4},\frac{1}{4},0$) x,x $-\frac{1}{4},\frac{1}{4}$ | (14) 2($\frac{1}{4},-\frac{1}{4},0$) x, $\bar{x}+\frac{1}{4},\frac{1}{4}$ | (15) 4 ⁻ (0,0, $\frac{1}{2}$) $\frac{1}{4},-\frac{1}{4},z$ | (16) 4 ⁺ (0,0, $\frac{1}{2}$) $\frac{1}{4},\frac{1}{4},z$ |
| (17) 4 ⁻ ($\frac{1}{2},0,0$) x, $\frac{1}{4},\frac{1}{4}$ | (18) 2(0, $\frac{1}{4},\frac{1}{4}$) $\frac{1}{4},y-\frac{1}{4},y$ | (19) 2(0, $-\frac{1}{4},\frac{1}{4}$) $\frac{1}{4},y+\frac{1}{4},\bar{y}$ | (20) 4 ⁺ ($\frac{1}{2},0,0$) x, $-\frac{1}{4},\frac{1}{4}$ |
| (21) 4 ⁺ $\frac{1}{2},y,0$ | (22) 2($\frac{1}{2},0,\frac{1}{2}$) x,0,x | (23) 4 ⁻ 0,y, $\frac{1}{2}$ | (24) 2 $\bar{x}+\frac{1}{2},0,x$ |
| (25) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$ | (26) a x,y, $\frac{1}{4}$ | (27) n($\frac{1}{2},0,\frac{1}{2}$) x,0,z | (28) c $\frac{1}{4},y,z$ |
| (29) $\bar{3}^+$ x $-\frac{1}{2},x-\frac{1}{2},x$; 0,0, $\frac{1}{2}$ | (30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$; 0,0, $\frac{1}{2}$ | (31) $\bar{3}^+$ x $+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$ | (32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{1}{2},-\frac{1}{2},0$ |
| (33) $\bar{3}^-$ x $+\frac{1}{2},x,x$; $\frac{1}{2},0,0$ | (34) $\bar{3}^-$ x $+\frac{1}{2},\bar{x}-1,\bar{x}$; 0, $-\frac{1}{2},\frac{1}{2}$ | (35) $\bar{3}^-$ $\bar{x}+\frac{1}{2},\bar{x}+1,x$; 0, $\frac{1}{2},\frac{1}{2}$ | (36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{2},0,0$ |
| (37) g($\frac{1}{4},-\frac{1}{4},\frac{1}{2}$) x $+\frac{1}{4},\bar{x},z$ | (38) g($\frac{1}{4},\frac{1}{4},\frac{1}{2}$) x $+\frac{1}{4},x,z$ | (39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ |
| (41) $\bar{4}^-$ x, $-\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ | (42) g($\frac{1}{2},-\frac{1}{4},\frac{1}{4}$) x,y $+\frac{1}{4},\bar{y}$ | (43) g($\frac{1}{2},\frac{1}{4},\frac{1}{4}$) x,y $-\frac{1}{4},y$ | (44) $\bar{4}^+$ x, $\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |
| (45) $\bar{4}^+$ 0,y, $\frac{1}{2}$; 0,0, $\frac{1}{2}$ | (46) m $\bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},0,0$ | (48) g($\frac{1}{2},0,\frac{1}{2}$) x,y,x |

For ($\frac{1}{2},\frac{1}{2},0$)+ set

- | | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) 2(0, $\frac{1}{2},0$) $\frac{1}{4},y,0$ | (4) 2($\frac{1}{2},0,0$) x, $\frac{1}{4},0$ |
| (5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $+\frac{1}{6},x+\frac{1}{3},x$ | (6) 3 ⁺ $\bar{x}+\frac{1}{2},x,\bar{x}$ | (7) 3 ⁺ x $+\frac{1}{2},\bar{x},\bar{x}$ | (8) 3 ⁺ ($\frac{1}{3},\frac{1}{3},-\frac{1}{3}$) $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ |
| (9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x $+\frac{1}{3},x+\frac{1}{6},x$ | (10) 3 ⁻ x, $\bar{x}+\frac{1}{2},\bar{x}$ | (11) 3 ⁻ ($-\frac{1}{3},\frac{1}{3},-\frac{1}{3}$) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) 3 ⁻ $\bar{x},x+\frac{1}{2},\bar{x}$ |
| (13) 2($\frac{1}{2},\frac{1}{2},0$) x,x,0 | (14) 2 x, $\bar{x}+\frac{1}{2},0$ | (15) 4 ⁻ $\frac{1}{2},0,z$ | (16) 4 ⁺ 0, $\frac{1}{2},z$ |
| (17) 4 ⁻ ($\frac{1}{2},0,0$) x, $\frac{1}{4},-\frac{1}{4}$ | (18) 2(0, $\frac{1}{4},\frac{1}{4}$) $\frac{1}{4},y+\frac{1}{4},y$ | (19) 2(0, $\frac{1}{4},-\frac{1}{4}$) $\frac{1}{4},y+\frac{1}{4},\bar{y}$ | (20) 4 ⁺ ($\frac{1}{2},0,0$) x, $\frac{1}{4},\frac{1}{4}$ |
| (21) 4 ⁺ (0, $\frac{1}{2},0$) $\frac{1}{4},y,-\frac{1}{4}$ | (22) 2($\frac{1}{4},0,\frac{1}{4}$) x $+\frac{1}{4},\frac{1}{4},x$ | (23) 4 ⁻ (0, $\frac{1}{2},0$) $\frac{1}{4},y,\frac{1}{4}$ | (24) 2($\frac{1}{4},0,-\frac{1}{4}$) $\bar{x}+\frac{1}{4},\frac{1}{4},x$ |
| (25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ | (26) n($\frac{1}{2},\frac{1}{2},0$) x,y,0 | (27) a x, $\frac{1}{4},z$ | (28) b $\frac{1}{4},y,z$ |
| (29) $\bar{3}^+$ x $+\frac{1}{2},x,x$; $\frac{1}{2},0,0$ | (30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; 0, $\frac{1}{2},\frac{1}{2}$ | (31) $\bar{3}^+$ x $-\frac{1}{2},\bar{x}+1,\bar{x}$; 0, $\frac{1}{2},-\frac{1}{2}$ | (32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x},x$; $\frac{1}{2},0,0$ |
| (33) $\bar{3}^-$ x,x $+\frac{1}{2},x$; 0, $\frac{1}{2},0$ | (34) $\bar{3}^-$ x $+1,\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,\frac{1}{2}$ | (35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; 0, $\frac{1}{2},0$ | (36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,-\frac{1}{2}$ |
| (37) m x $+\frac{1}{2},\bar{x},z$ | (38) g($\frac{1}{2},\frac{1}{2},0$) x,x,z | (39) $\bar{4}^-$ 0, $\frac{1}{2},z$; 0, $\frac{1}{2},0$ | (40) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,0$ |
| (41) $\bar{4}^-$ x, $\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (42) g($\frac{1}{2},\frac{1}{4},-\frac{1}{4}$) x,y $+\frac{1}{4},\bar{y}$ | (43) g($\frac{1}{2},\frac{1}{4},\frac{1}{4}$) x,y $+\frac{1}{4},y$ | (44) $\bar{4}^+$ x, $\frac{1}{4},-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ |
| (45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (46) g($\frac{1}{4},\frac{1}{2},-\frac{1}{4}$) $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ | (48) g($\frac{1}{4},\frac{1}{2},\frac{1}{4}$) x $+\frac{1}{4},y,x$ |

$Fm\bar{3}c$

O_h^6

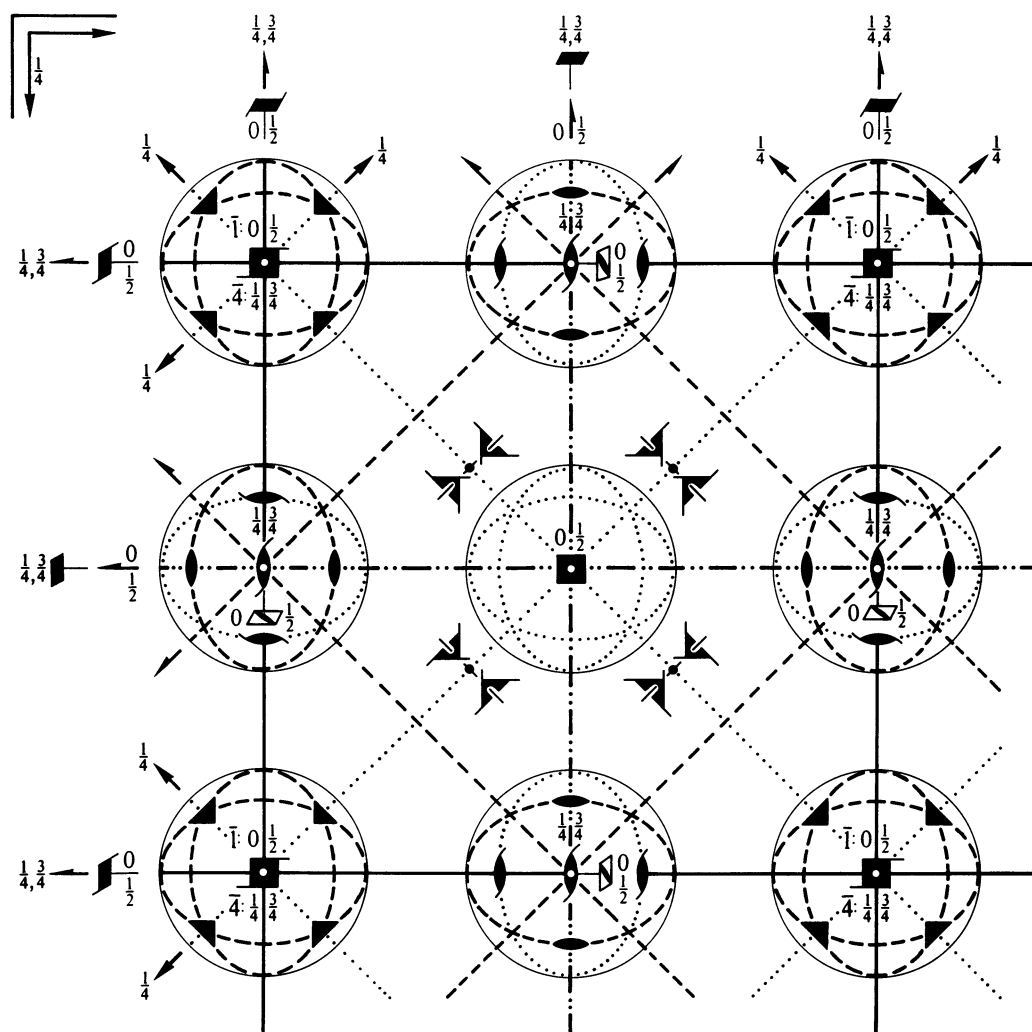
$m\bar{3}m$

Cubic

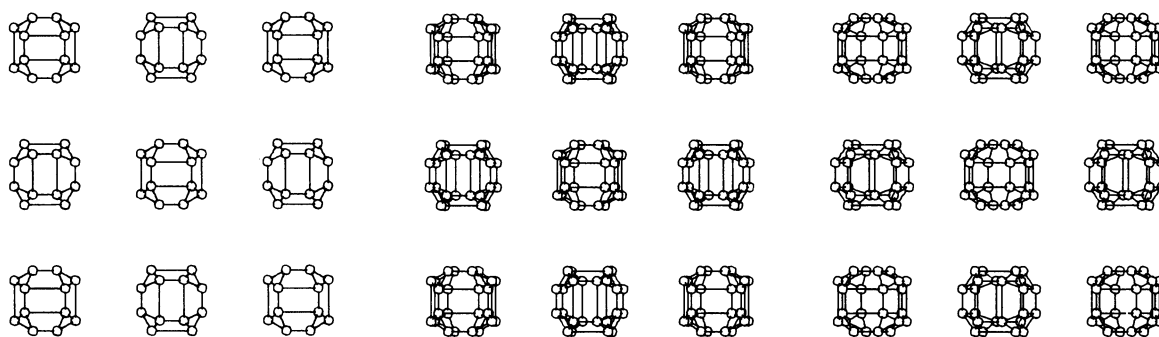
No. 226

$F 4/m \bar{3} 2/c$

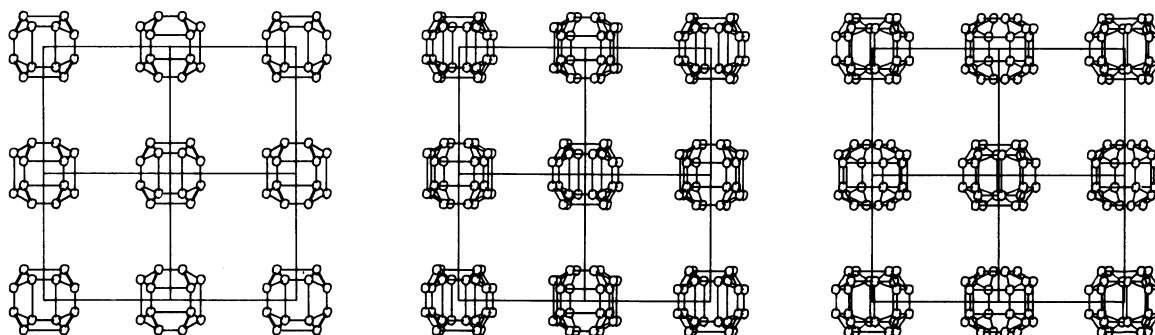
Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq \frac{1}{4}$; $y \leq \min(x, \frac{1}{2} - x)$; $z \leq y$
Vertices $0, 0, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

(given on page 695)

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0, 0, 0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	h, k, l permutable General:

192	j	1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$ (26) x, y, \bar{z} (30) \bar{z}, x, y (34) y, \bar{z}, x (38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (46) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (27) x, \bar{y}, z (31) z, x, \bar{y} (35) \bar{y}, z, x (39) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (28) \bar{x}, \bar{y}, z (32) z, \bar{x}, y (36) y, z, \bar{x} (40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (44) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	hkl : $h + k = 2n$ and $h + l, k + l = 2n$ $0kl$: $k, l = 2n$ hhl : $h, l = 2n$ $h00$: $h = 2n$
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Special: as above, plus

96	i	$m \dots$	$0, y, z$ $z, 0, y$ $y, z, 0$ $y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y}, z$ $z, 0, \bar{y}$ $\bar{y}, z, 0$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, y, \bar{z}$ $\bar{z}, 0, y$ $y, \bar{z}, 0$ $y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y}, \bar{z}$ $\bar{z}, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
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96	h	$\dots 2$	$\frac{1}{4}, y, y$ $\bar{y}, \frac{3}{4}, y$ $\frac{3}{4}, \bar{y}, \bar{y}$ $y, \frac{1}{4}, \bar{y}$	$\frac{3}{4}, \bar{y}, y$ $\bar{y}, \frac{1}{4}, \bar{y}$ $\frac{1}{4}, y, \bar{y}$ $y, \frac{3}{4}, y$	$\frac{3}{4}, y, \bar{y}$ $y, y, \frac{1}{4}$ $\frac{1}{4}, \bar{y}, y$ $\bar{y}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{3}{4}$ $\frac{3}{4}, y, y$ $y, \bar{y}, \frac{1}{4}$	$y, \frac{1}{4}, y$ $y, \bar{y}, \frac{3}{4}$ $\bar{y}, \frac{3}{4}, \bar{y}$ $\bar{y}, y, \frac{1}{4}$	$y, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{4}$ $\bar{y}, \frac{1}{4}, y$ $y, y, \frac{3}{4}$	hkl : $h = 2n$
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64	g	$\dots 3 \dots$	x, x, x \bar{x}, x, \bar{x} $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{x}$ x, \bar{x}, x $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, \bar{x}, x x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ x, x, \bar{x} \bar{x}, x, x $x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$				hkl : $h = 2n$
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48	f	$4 \dots$	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x$	hkl : $h = 2n$
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48	e	$mm2 \dots$	$x, 0, 0$ $0, 0, x$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $0, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0, \bar{x}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$		hkl : $h = 2n$
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24	d	$4/m \dots$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	hkl : $h = 2n$
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24	c	$\bar{4}m \dots 2$	$\frac{1}{4}, 0, 0$	$\frac{3}{4}, 0, 0$	$0, \frac{1}{4}, 0$	$0, \frac{3}{4}, 0$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$	hkl : $h = 2n$
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8	b	$m\bar{3} \dots$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					hkl : $h = 2n$
---	-----	------------------	-----------	---	--	--	--	--	------------------

8	a	432	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$					hkl : $h = 2n$
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Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0, 0, z

Along [111] $p6mm$
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at x, x, 0

Maximal non-isomorphic subgroups

I	<p>[2] $F\bar{4}3c$ (219) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+</p> <p>[2] $F432$ (209) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+</p> <p>[2] $Fm\bar{3}1$ ($Fm\bar{3}$, 202) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+</p> <p>{ [3] $F4_2/m12/n$ ($I4/mcm$, 140) (1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+</p> <p>{ [3] $F4_2/m12/n$ ($I4/mcm$, 140) (1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+</p> <p>{ [3] $F4_2/m12/n$ ($I4/mcm$, 140) (1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+</p> <p>{ [4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167) (1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+</p> <p>{ [4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167) (1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+</p> <p>{ [4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167) (1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+</p> <p>{ [4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167) (1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+</p>
IIa	<p>{ [4] $Pm\bar{3}n$ (223) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48</p> <p>{ [4] $Pm\bar{3}n$ (223) 1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0, \frac{1}{2}, \frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$</p> <p>{ [4] $Pm\bar{3}n$ (223) 1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2}, \frac{1}{2}, 0)$</p> <p>{ [4] $Pm\bar{3}n$ (223) 1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0, \frac{1}{2}, \frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2}, \frac{1}{2}, 0)$</p> <p>{ [4] $Pn\bar{3}n$ (222) 1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2}, \frac{1}{2}, 0)$</p> <p>{ [4] $Pn\bar{3}n$ (222) 1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2}, \frac{1}{2}, 0)$</p> <p>{ [4] $Pn\bar{3}n$ (222) 1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2}, \frac{1}{2}, 0)$</p> <p>{ [4] $Pn\bar{3}n$ (222) 1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2}, \frac{1}{2}, 0)$</p>
IIb	<p>none</p>

Maximal isomorphic subgroups of lowest index

IIc [27] $Fm\bar{3}c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (226)

Minimal non-isomorphic supergroups

I none

II [2] $Pm\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (221)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--|--|--|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) 2($\frac{1}{2},\frac{1}{2},0$) x,x, $\frac{1}{4}$ | (14) 2 x, $\bar{x}+\frac{1}{2},\frac{1}{4}$ | (15) 4 ⁻ (0,0, $\frac{1}{2}$) $\frac{1}{2},0,z$ | (16) 4 ⁺ (0,0, $\frac{1}{2}$) 0, $\frac{1}{2},z$ |
| (17) 4 ⁻ ($\frac{1}{2},0,0$) x, $\frac{1}{2},0$ | (18) 2(0, $\frac{1}{2},\frac{1}{2}$) $\frac{1}{4},y,y$ | (19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$ | (20) 4 ⁺ ($\frac{1}{2},0,0$) x,0, $\frac{1}{2}$ |
| (21) 4 ⁺ (0, $\frac{1}{2},0$) $\frac{1}{2},y,0$ | (22) 2($\frac{1}{2},0,\frac{1}{2}$) x, $\frac{1}{4},x$ | (23) 4 ⁻ (0, $\frac{1}{2},0$) 0,y, $\frac{1}{2}$ | (24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$ |
| (25) $\bar{1}$ 0,0,0 | (26) m x,y,0 | (27) m x,0,z | (28) m 0,y,z |
| (29) $\bar{3}^+$ x,x,x; 0,0,0 | (30) $\bar{3}^+$ \bar{x},x,\bar{x} ; 0,0,0 | (31) $\bar{3}^+$ x, \bar{x},\bar{x} ; 0,0,0 | (32) $\bar{3}^+$ \bar{x},\bar{x},x ; 0,0,0 |
| (33) $\bar{3}^-$ x,x,x; 0,0,0 | (34) $\bar{3}^-$ x, \bar{x},\bar{x} ; 0,0,0 | (35) $\bar{3}^-$ \bar{x},\bar{x},x ; 0,0,0 | (36) $\bar{3}^-$ \bar{x},x,\bar{x} ; 0,0,0 |
| (37) c x+ $\frac{1}{2},\bar{x},z$ | (38) n($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) x,x,z | (39) $\bar{4}^-$ 0, $\frac{1}{2},z$; 0, $\frac{1}{2},\frac{1}{4}$ | (40) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$ |
| (41) $\bar{4}^-$ x,0, $\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$ | (42) a x,y+ $\frac{1}{2},\bar{y}$ | (43) n($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) x,y,y | (44) $\bar{4}^+$ x, $\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$ |
| (45) $\bar{4}^+$ 0,y, $\frac{1}{2}$; 0, $\frac{1}{4},\frac{1}{2}$ | (46) b $\bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$ | (48) n($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) x,y,x |

For (0, $\frac{1}{2},\frac{1}{2}$)+ set

- | | | | |
|---|---|--|--|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) 0, $\frac{1}{4},z$ | (3) 2(0, $\frac{1}{2},0$) 0,y, $\frac{1}{4}$ | (4) 2 x, $\frac{1}{4},\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x- $\frac{1}{3},x-\frac{1}{6},x$ | (6) 3 ⁺ $\bar{x},x+\frac{1}{2},\bar{x}$ | (7) 3 ⁺ (- $\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x+ $\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) 3 ⁺ $\bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x- $\frac{1}{6},x+\frac{1}{6},x$ | (10) 3 ⁻ (- $\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x+ $\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) 3 ⁻ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ | (12) 3 ⁻ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ |
| (13) 2($\frac{1}{4},\frac{1}{4},0$) x,x- $\frac{1}{4},0$ | (14) 2($\frac{1}{4},-\frac{1}{4},0$) x, $\bar{x}+\frac{1}{4},0$ | (15) 4 ⁻ $\frac{1}{4},-\frac{1}{4},z$ | (16) 4 ⁺ $\frac{1}{4},\frac{1}{4},z$ |
| (17) 4 ⁻ ($\frac{1}{2},0,0$) x,0,0 | (18) 2 $\frac{1}{4},y,y$ | (19) 2 $\frac{1}{4},y,\bar{y}$ | (20) 4 ⁺ ($\frac{1}{2},0,0$) x,0,0 |
| (21) 4 ⁺ $\frac{1}{4},y,-\frac{1}{4}$ | (22) 2($\frac{1}{4},0,\frac{1}{4}$) x+ $\frac{1}{4},0,x$ | (23) 4 ⁻ $\frac{1}{4},y,\frac{1}{4}$ | (24) 2($\frac{1}{4},0,-\frac{1}{4}$) $\bar{x}+\frac{1}{4},0,x$ |
| (25) $\bar{1}$ 0, $\frac{1}{4},\frac{1}{4}$ | (26) b x,y, $\frac{1}{4}$ | (27) c x, $\frac{1}{4},z$ | (28) n(0, $\frac{1}{2},\frac{1}{2}$) 0,y,z |
| (29) $\bar{3}^+$ x,x+ $\frac{1}{2},x$; 0, $\frac{1}{2},0$ | (30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; - $\frac{1}{2},0,\frac{1}{2}$ | (31) $\bar{3}^+$ x, $\bar{x}+\frac{1}{2},\bar{x}$; 0, $\frac{1}{2},0$ | (32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{1}{2},0,\frac{1}{2}$ |
| (33) $\bar{3}^-$ x- $\frac{1}{2},x-\frac{1}{2},x$; 0,0, $\frac{1}{2}$ | (34) $\bar{3}^-$ x+ $\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; 0,0, $\frac{1}{2}$ | (35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; - $\frac{1}{2},\frac{1}{2},0$ | (36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$ |
| (37) g($\frac{1}{4},-\frac{1}{4},0$) x+ $\frac{1}{4},\bar{x},z$ | (38) g($\frac{1}{4},\frac{1}{4},0$) x+ $\frac{1}{4},x,z$ | (39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$ | (40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$ |
| (41) $\bar{4}^-$ x,0,0; $\frac{1}{4},0,0$ | (42) a x,y, \bar{y} | (43) a x,y,y | (44) $\bar{4}^+$ x,0,0; $\frac{1}{4},0,0$ |
| (45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$ | (46) g($\frac{1}{4},0,-\frac{1}{4}$) $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},0,-\frac{1}{4}$ | (48) g($\frac{1}{4},0,\frac{1}{4}$) x+ $\frac{1}{4},y,x$ |

For ($\frac{1}{2},0,\frac{1}{2}$)+ set

- | | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4},0,z$ | (3) 2 $\frac{1}{4},y,\frac{1}{4}$ | (4) 2($\frac{1}{2},0,0$) x,0, $\frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x+ $\frac{1}{6},x-\frac{1}{6},x$ | (6) 3 ⁺ ($\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ | (7) 3 ⁺ x+ $\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) 3 ⁺ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ |
| (9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x- $\frac{1}{6},x-\frac{1}{6},x$ | (10) 3 ⁻ x+ $\frac{1}{2},\bar{x},\bar{x}$ | (11) 3 ⁻ $\bar{x}+\frac{1}{2},\bar{x},x$ | (12) 3 ⁻ (- $\frac{1}{3},-\frac{1}{3},\frac{1}{3}$) $\bar{x}-\frac{1}{6},x+\frac{1}{6},\bar{x}$ |
| (13) 2($\frac{1}{4},\frac{1}{4},0$) x,x+ $\frac{1}{4},0$ | (14) 2(- $\frac{1}{4},\frac{1}{4},0$) x, $\bar{x}+\frac{1}{4},0$ | (15) 4 ⁻ $\frac{1}{4},\frac{1}{4},z$ | (16) 4 ⁺ - $\frac{1}{4},\frac{1}{4},z$ |
| (17) 4 ⁻ x, $\frac{1}{4},-\frac{1}{4}$ | (18) 2(0, $\frac{1}{4},\frac{1}{4}$) 0,y+ $\frac{1}{4},y$ | (19) 2(0, $\frac{1}{4},-\frac{1}{4}$) 0,y+ $\frac{1}{4},\bar{y}$ | (20) 4 ⁺ x, $\frac{1}{4},\frac{1}{4}$ |
| (21) 4 ⁺ (0, $\frac{1}{2},0$) 0,y,0 | (22) 2 x, $\frac{1}{4},x$ | (23) 4 ⁻ (0, $\frac{1}{2},0$) 0,y,0 | (24) 2 $\bar{x},\frac{1}{4},x$ |
| (25) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$ | (26) a x,y, $\frac{1}{4}$ | (27) n($\frac{1}{2},0,\frac{1}{2}$) x,0,z | (28) c $\frac{1}{4},y,z$ |
| (29) $\bar{3}^+$ x- $\frac{1}{2},x-\frac{1}{2},x$; 0,0, $\frac{1}{2}$ | (30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$; 0,0, $\frac{1}{2}$ | (31) $\bar{3}^+$ x+ $\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$ | (32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{1}{2},-\frac{1}{2},0$ |
| (33) $\bar{3}^-$ x+ $\frac{1}{2},x,x$; $\frac{1}{2},0,0$ | (34) $\bar{3}^-$ x+ $\frac{1}{2},\bar{x}-1,\bar{x}$; 0,- $\frac{1}{2},\frac{1}{2}$ | (35) $\bar{3}^-$ $\bar{x}+\frac{1}{2},\bar{x}+1,x$; 0, $\frac{1}{2},\frac{1}{2}$ | (36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{2},0,0$ |
| (37) g(- $\frac{1}{4},\frac{1}{4},0$) x+ $\frac{1}{4},\bar{x},z$ | (38) g($\frac{1}{4},\frac{1}{4},0$) x- $\frac{1}{4},x,z$ | (39) $\bar{4}^-$ - $\frac{1}{4},\frac{1}{4},z$; - $\frac{1}{4},\frac{1}{4},0$ | (40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$ |
| (41) $\bar{4}^-$ x, $\frac{1}{4},\frac{1}{4}$; 0, $\frac{1}{4},\frac{1}{4}$ | (42) g(0, $\frac{1}{4},-\frac{1}{4}$) x,y+ $\frac{1}{4},\bar{y}$ | (43) g(0, $\frac{1}{4},\frac{1}{4}$) x,y+ $\frac{1}{4},y$ | (44) $\bar{4}^+$ x, $\frac{1}{4},-\frac{1}{4}$; 0, $\frac{1}{4},-\frac{1}{4}$ |
| (45) $\bar{4}^+$ 0,y,0; 0, $\frac{1}{4},0$ | (46) b \bar{x},y,x | (47) $\bar{4}^-$ 0,y,0; 0, $\frac{1}{4},0$ | (48) b x,y,x |

For ($\frac{1}{2},\frac{1}{2},0$)+ set

- | | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) 2(0, $\frac{1}{2},0$) $\frac{1}{4},y,0$ | (4) 2($\frac{1}{2},0,0$) x, $\frac{1}{4},0$ |
| (5) 3 ⁺ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x+ $\frac{1}{6},x+\frac{1}{3},x$ | (6) 3 ⁺ $\bar{x}+\frac{1}{2},x,\bar{x}$ | (7) 3 ⁺ x+ $\frac{1}{2},\bar{x},\bar{x}$ | (8) 3 ⁺ ($\frac{1}{3},\frac{1}{3},-\frac{1}{3}$) $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ |
| (9) 3 ⁻ ($\frac{1}{3},\frac{1}{3},\frac{1}{3}$) x+ $\frac{1}{3},x+\frac{1}{6},x$ | (10) 3 ⁻ x, $\bar{x}+\frac{1}{2},\bar{x}$ | (11) 3 ⁻ (- $\frac{1}{3},\frac{1}{3},-\frac{1}{3}$) $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) 3 ⁻ $\bar{x},x+\frac{1}{2},\bar{x}$ |
| (13) 2 x,x, $\frac{1}{4}$ | (14) 2 x, $\bar{x},\frac{1}{4}$ | (15) 4 ⁻ (0,0, $\frac{1}{2}$) 0,0,z | (16) 4 ⁺ (0,0, $\frac{1}{2}$) 0,0,z |
| (17) 4 ⁻ x, $\frac{1}{4},\frac{1}{4}$ | (18) 2(0, $\frac{1}{4},\frac{1}{4}$) 0,y- $\frac{1}{4},y$ | (19) 2(0,- $\frac{1}{4},\frac{1}{4}$) 0,y+ $\frac{1}{4},\bar{y}$ | (20) 4 ⁺ x,- $\frac{1}{4},\frac{1}{4}$ |
| (21) 4 ⁺ $\frac{1}{4},y,\frac{1}{4}$ | (22) 2($\frac{1}{4},0,\frac{1}{4}$) x- $\frac{1}{4},0,x$ | (23) 4 ⁻ - $\frac{1}{4},y,\frac{1}{4}$ | (24) 2(- $\frac{1}{4},0,\frac{1}{4}$) $\bar{x}+\frac{1}{4},0,x$ |
| (25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ | (26) n($\frac{1}{2},\frac{1}{2},0$) x,y,0 | (27) a x, $\frac{1}{4},z$ | (28) b $\frac{1}{4},y,z$ |
| (29) $\bar{3}^+$ x+ $\frac{1}{2},x,x$; $\frac{1}{2},0,0$ | (30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; 0, $\frac{1}{2},\frac{1}{2}$ | (31) $\bar{3}^+$ x- $\frac{1}{2},\bar{x}+1,\bar{x}$; 0, $\frac{1}{2},-\frac{1}{2}$ | (32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x},x$; $\frac{1}{2},0,0$ |
| (33) $\bar{3}^-$ x,x+ $\frac{1}{2},x$; 0, $\frac{1}{2},0$ | (34) $\bar{3}^-$ x+1, $\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,\frac{1}{2}$ | (35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; 0, $\frac{1}{2},0$ | (36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,-\frac{1}{2}$ |
| (37) c x, \bar{x},z | (38) c x,x,z | (39) $\bar{4}^-$ 0,0,z; 0,0, $\frac{1}{4}$ | (40) $\bar{4}^+$ 0,0,z; 0,0, $\frac{1}{4}$ |
| (41) $\bar{4}^-$ x,- $\frac{1}{4},\frac{1}{4}$; 0,- $\frac{1}{4},\frac{1}{4}$ | (42) g(0,- $\frac{1}{4},\frac{1}{4}$) x,y+ $\frac{1}{4},\bar{y}$ | (43) g(0, $\frac{1}{4},\frac{1}{4}$) x,y- $\frac{1}{4},y$ | (44) $\bar{4}^+$ x, $\frac{1}{4},\frac{1}{4}$; 0, $\frac{1}{4},\frac{1}{4}$ |
| (45) $\bar{4}^+$ - $\frac{1}{4},y,\frac{1}{4}$; - $\frac{1}{4},0,\frac{1}{4}$ | (46) g(- $\frac{1}{4},0,\frac{1}{4}$) $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$ | (48) g($\frac{1}{4},0,\frac{1}{4}$) x- $\frac{1}{4},y,x$ |

$Fd\bar{3}m$

O_h^7

$m\bar{3}m$

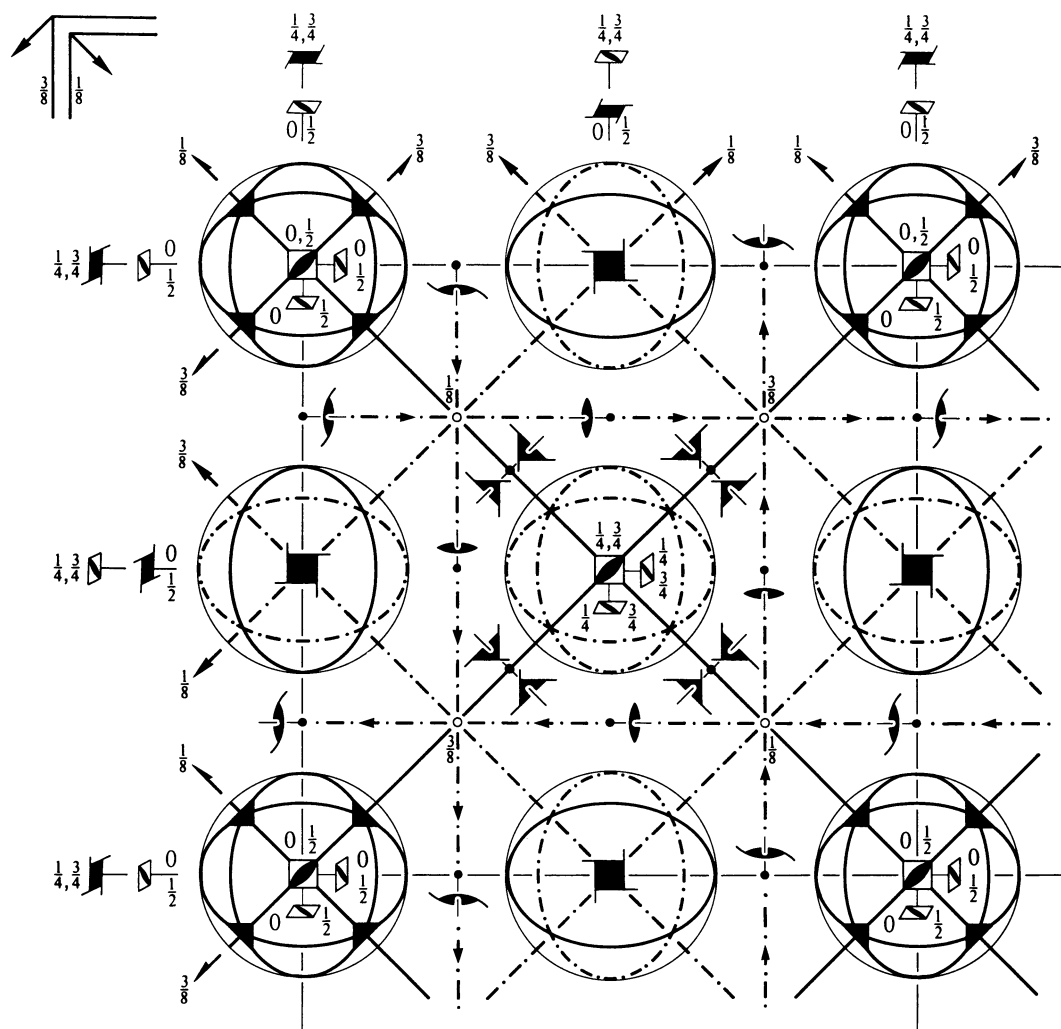
Cubic

No. 227

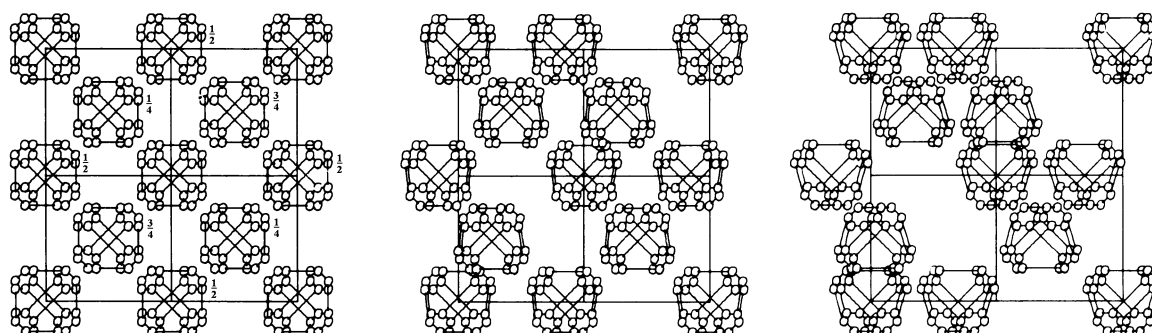
$F 4_1/d \bar{3} 2/m$

Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at $\bar{4}3m$, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{8}; -\frac{1}{8} \leq z \leq \frac{1}{8}; y \leq \min(\frac{1}{2}-x, x); -y \leq z \leq y$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{3}{8}, \frac{1}{8}, \frac{1}{8} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8} \quad \frac{3}{8}, \frac{1}{8}, -\frac{1}{8} \quad \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$

Symmetry operations

(given on page 699)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions					
	$(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ $(\frac{1}{2}, 0, \frac{1}{2})+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$	h, k, l permutable General:					
192 <i>i</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$ (21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$ (25) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (29) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}$ (33) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ (37) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$ (10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ (14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$ (22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$ (26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (30) $\bar{z} + \frac{3}{4}, x + \frac{1}{4}, y + \frac{3}{4}$ (34) $y + \frac{3}{4}, \bar{z} + \frac{3}{4}, x + \frac{1}{4}$ (38) y, x, z (42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y}$ (46) $\bar{z}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$ (15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$ (19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$ (23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$ (27) $x + \frac{3}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{4}$ (31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{3}{4}$ (35) $\bar{y} + \frac{3}{4}, z + \frac{1}{4}, x + \frac{3}{4}$ (39) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (43) x, z, y (47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$ (12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ (16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ (20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$ (24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ (28) $\bar{x} + \frac{3}{4}, y + \frac{1}{4}, z + \frac{3}{4}$ (32) $z + \frac{3}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{4}$ (36) $y + \frac{1}{4}, z + \frac{3}{4}, \bar{x} + \frac{3}{4}$ (40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (44) $\bar{x}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (48) z, y, x	$hkl : h + k = 2n$ and $h + l, k + l = 2n$ $OkI : k + l = 4n$ and $k, l = 2n$ $hhl : h + l = 2n$ $h00 : h = 4n$		
96 <i>h</i> .. 2	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{1}{8}, y$ $y, \bar{y} + \frac{1}{4}, \frac{1}{8}$ $\frac{1}{8}, \bar{y} + \frac{1}{4}, y$ $y, \frac{1}{8}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, y, \frac{1}{8}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \frac{7}{8}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{7}{8}$ $\frac{3}{8}, y + \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{8}, y + \frac{3}{4}$ $y + \frac{3}{4}, y + \frac{1}{2}, \frac{3}{8}$	$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$ $y + \frac{3}{4}, \frac{3}{8}, y + \frac{1}{2}$ $y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{8}$ $\frac{7}{8}, \bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{7}{8}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{7}{8}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$ $y + \frac{1}{4}, \frac{5}{8}, \bar{y}$ $\bar{y}, y + \frac{1}{4}, \frac{5}{8}$ $\frac{5}{8}, y + \frac{1}{4}, \bar{y}$ $\bar{y}, \frac{5}{8}, y + \frac{1}{4}$ $y + \frac{1}{4}, \bar{y}, \frac{5}{8}$	no extra conditions 		
96 <i>g</i> .. <i>m</i>	x, x, z z, x, x x, z, x $x + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$ $x + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{3}{4}$ $z + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, x + \frac{1}{4}$ $z + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $\bar{z}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$ $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ $\bar{z} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	$x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $\bar{x}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, x + \frac{3}{4}$ $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	no extra conditions		
48 <i>f</i> 2. <i>mm</i>	$x, 0, 0$ $\frac{3}{4}, x + \frac{1}{4}, \frac{3}{4}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{1}{4}$	$0, x, 0$ $x + \frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$0, 0, x$ $\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x + \frac{3}{4}$	$hkl : h = 2n + 1$ or $h + k + l = 4n$
32 <i>e</i> . 3 <i>m</i>	x, x, x $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$ $x + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ $\bar{x} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$				no extra conditions	
16 <i>d</i> . $\bar{3}m$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{1}{8}$ $\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{3}{8}$ $\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{3}{8}, \frac{7}{8}$ $\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$		$hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$	
16 <i>c</i> . $\bar{3}m$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$		$hkl : h = 2n + 1$ or $h + k + l = 4n$	
8 <i>b</i> $\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$				$hkl : h = 2n + 1$ or $h + k + l = 4n$	
8 <i>a</i> $\bar{4}3m$	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$					

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$

Origin at 0, 0, z

Along [111] $p6mm$

$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$

Origin at x, x, x

Along [110] $c2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Origin at x, x, $\frac{1}{8}$

ORIGIN CHOICE 1

Maximal non-isomorphic subgroups

I	[2] $F \bar{4} 3 m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F 4_1 3 2$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $F d \bar{3} 1$ ($F d \bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	{ [3] $F 4_1/d 1 2/m$ ($I 4_1/am d$, 141)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	{ [3] $F 4_1/d 1 2/m$ ($I 4_1/am d$, 141)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	{ [3] $F 4_1/d 1 2/m$ ($I 4_1/am d$, 141)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F d \bar{3} m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (227)

Minimal non-isomorphic supergroups

I none

II [2] $P n \bar{3} m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ | (4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$ |
| (5) $3^+ x,x,x$ | (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ | (7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ |
| (9) $3^- x,x,x$ | (10) $3^- x,\bar{x}+\frac{1}{2},\bar{x}$ | (11) $3^- \bar{x}+\frac{1}{2},\bar{x},x$ | (12) $3^- \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$ | (14) $2 x,\bar{x}+\frac{1}{4},\frac{1}{8}$ | (15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},\frac{1}{4},z$ | (16) $4^+(0,0,\frac{1}{4})$ $0,\frac{3}{4},z$ |
| (17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},\frac{1}{4}$ | (18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y+\frac{1}{4},y$ | (19) $2 \frac{1}{8},y+\frac{1}{4},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{3}{4}$ |
| (21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{4},y,0$ | (22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{3}{8},x$ | (23) $4^-(0,\frac{3}{4},0)$ $\frac{1}{4},y,\frac{1}{2}$ | (24) $2 \bar{x}+\frac{1}{4},\frac{1}{8},x$ |
| (25) $\bar{1} \frac{1}{8},\frac{1}{8},\frac{1}{8}$ | (26) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{3}{8}$ | (27) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$ | (28) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{3}{8},y,z$ |
| (29) $\bar{3}^+ x,x,x$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ | (30) $\bar{3}^+ \bar{x}-1,x+1,\bar{x}$; $-\frac{1}{8},\frac{1}{8},\frac{7}{8}$ | (31) $\bar{3}^+ x,\bar{x}+1,\bar{x}$; $\frac{1}{8},\frac{7}{8},-\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x}+1,\bar{x},x$; $\frac{7}{8},-\frac{1}{8},\frac{1}{8}$ |
| (33) $\bar{3}^- x,x,x$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ | (34) $\bar{3}^- x+\frac{3}{2},\bar{x}-1,\bar{x}$; $\frac{5}{8},-\frac{1}{8},\frac{7}{8}$ | (35) $\bar{3}^- \bar{x}+\frac{1}{2},\bar{x}+\frac{3}{2},x$; $-\frac{1}{8},\frac{7}{8},\frac{5}{8}$ | (36) $\bar{3}^- \bar{x}+1,x+\frac{1}{2},\bar{x}$; $\frac{7}{8},\frac{5}{8},-\frac{1}{8}$ |
| (37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$ | (38) $m x,x,z$ | (39) $\bar{4}^- -\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (40) $\bar{4}^+ \frac{1}{2},0,z$; $\frac{1}{2},0,0$ |
| (41) $\bar{4}^- x,-\frac{1}{4},\frac{1}{4}; \frac{1}{4},-\frac{1}{4},\frac{1}{4}$ | (42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$ | (43) $m x,y,y$ | (44) $\bar{4}^+ x,\frac{1}{2},0; 0,\frac{1}{2},0$ |
| (45) $\bar{4}^+ 0,y,\frac{1}{2}; 0,0,\frac{1}{2}$ | (46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^- \frac{1}{4},y,-\frac{1}{4}; \frac{1}{4},\frac{1}{4},-\frac{1}{4}$ | (48) $m x,y,x$ |

For (0, $\frac{1}{2},\frac{1}{2}$)+ set

- | | | | |
|--|---|--|---|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) 2 0,0,z | (3) 2 $\frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$ | (6) $3^+ \bar{x}+\frac{1}{2},x,\bar{x}$ | (7) $3^+ x,\bar{x},\bar{x}$ | (8) $3^+ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$ | (10) $3^- x+\frac{1}{2},\bar{x},\bar{x}$ | (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^- \bar{x},x,\bar{x}$ |
| (13) $2(\frac{3}{4},\frac{3}{4},0)$ $x,x,\frac{1}{8}$ | (14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$ | (15) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},0,z$ | (16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$ |
| (17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},-\frac{1}{4}$ | (18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$ | (19) $2 \frac{1}{8},y+\frac{3}{4},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{1}{4}$ |
| (21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$ | (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},x$ | (23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$ | (24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$ |
| (25) $\bar{1} \frac{1}{8},\frac{3}{8},\frac{3}{8}$ | (26) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,\frac{1}{8}$ | (27) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$ | (28) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{3}{8},y,z$ |
| (29) $\bar{3}^+ x,x+\frac{1}{2},x$; $\frac{1}{8},\frac{5}{8},\frac{1}{8}$ | (30) $\bar{3}^+ \bar{x}-1,x+\frac{3}{2},\bar{x}$; $-\frac{1}{8},\frac{5}{8},\frac{7}{8}$ | (31) $\bar{3}^+ x,\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{8},\frac{3}{8},-\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x}+1,\bar{x}-\frac{1}{2},x$; $\frac{7}{8},-\frac{5}{8},\frac{1}{8}$ |
| (33) $\bar{3}^- x-\frac{1}{2},x-\frac{1}{2},x$; $\frac{1}{8},\frac{1}{8},\frac{5}{8}$ | (34) $\bar{3}^- x+1,\bar{x}-\frac{3}{2},\bar{x}$; $\frac{1}{8},-\frac{5}{8},\frac{7}{8}$ | (35) $\bar{3}^- \bar{x},\bar{x}+1,x$; $-\frac{1}{8},\frac{7}{8},\frac{1}{8}$ | (36) $\bar{3}^- \bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ |
| (37) $m x+\frac{1}{2},\bar{x},z$ | (38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x-\frac{1}{4},x,z$ | (39) $\bar{4}^- 0,0,z; 0,0,0$ | (40) $\bar{4}^+ \frac{1}{4},-\frac{1}{4},z; \frac{1}{4},-\frac{1}{4},\frac{1}{4}$ |
| (41) $\bar{4}^- x,\frac{1}{4},\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$ | (43) $g(0,\frac{1}{2},\frac{1}{2})$ x,y,y | (44) $\bar{4}^+ x,0,0; 0,0,0$ |
| (45) $\bar{4}^+ \frac{1}{4},y,\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (46) $m \bar{x},y,x$ | (47) $\bar{4}^- \frac{1}{2},y,0; \frac{1}{2},0,0$ | (48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x-\frac{1}{4},y,x$ |

For ($\frac{1}{2},0,\frac{1}{2}$)+ set

- | | | | |
|--|---|---|---|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ | (4) 2 $x,0,0$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$ | (6) $3^+ \bar{x},x,\bar{x}$ | (7) $3^+ x+\frac{1}{2},\bar{x},\bar{x}$ | (8) $3^+ \bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$ | (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^- \bar{x},\bar{x},x$ | (12) $3^- \bar{x},x+\frac{1}{2},\bar{x}$ |
| (13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,\frac{1}{8}$ | (14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$ | (15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$ | (16) $4^+(0,0,\frac{3}{4})$ $-\frac{1}{4},\frac{1}{2},z$ |
| (17) $4^-(\frac{1}{4},0,0)$ $x,\frac{1}{4},0$ | (18) $2(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,y$ | (19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$ | (20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$ |
| (21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{4},y,0$ | (22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$ | (23) $4^-(0,\frac{3}{4},0)$ $-\frac{1}{4},y,\frac{1}{2}$ | (24) $2 \bar{x}+\frac{3}{4},\frac{1}{8},x$ |
| (25) $\bar{1} \frac{3}{8},\frac{1}{8},\frac{3}{8}$ | (26) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,\frac{1}{8}$ | (27) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$ | (28) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,z$ |
| (29) $\bar{3}^+ x-\frac{1}{2},x-\frac{1}{2},x$; $\frac{1}{8},\frac{1}{8},\frac{5}{8}$ | (30) $\bar{3}^+ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$; $-\frac{1}{8},\frac{1}{8},\frac{3}{8}$ | (31) $\bar{3}^+ x-\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{8},\frac{7}{8},-\frac{5}{8}$ | (32) $\bar{3}^+ \bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x$; $\frac{7}{8},-\frac{1}{8},\frac{5}{8}$ |
| (33) $\bar{3}^- x+\frac{1}{2},x,x$; $\frac{5}{8},\frac{1}{8},\frac{1}{8}$ | (34) $\bar{3}^- x+1,\bar{x}-1,\bar{x}$; $\frac{1}{8},-\frac{1}{8},\frac{7}{8}$ | (35) $\bar{3}^- \bar{x},\bar{x}+\frac{1}{2},x$; $-\frac{1}{8},\frac{3}{8},\frac{1}{8}$ | (36) $\bar{3}^- \bar{x}+\frac{3}{2},x-\frac{1}{2},\bar{x}$; $\frac{7}{8},\frac{1}{8},-\frac{5}{8}$ |
| (37) $m x,\bar{x},z$ | (38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},x,z$ | (39) $\bar{4}^- 0,\frac{1}{2},z; 0,\frac{1}{2},0$ | (40) $\bar{4}^+ \frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},\frac{1}{4}$ |
| (41) $\bar{4}^- x,0,0; 0,0,0$ | (42) $m x,y+\frac{1}{2},\bar{y}$ | (43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$ | (44) $\bar{4}^+ x,\frac{1}{4},-\frac{1}{4}; \frac{1}{4},\frac{1}{4},-\frac{1}{4}$ |
| (45) $\bar{4}^+ 0,y,0; 0,0,0$ | (46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^- \frac{1}{4},y,\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (48) $g(\frac{1}{2},0,\frac{1}{2})$ x,y,x |

For ($\frac{1}{2},\frac{1}{2},0$)+ set

- | | | | |
|---|---|---|--|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ | (3) 2 0,y,0 | (4) 2 $x,\frac{1}{4},\frac{1}{4}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$ | (6) $3^+ \bar{x},x+\frac{1}{2},\bar{x}$ | (7) $3^+ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+ \bar{x},\bar{x},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$ | (10) $3^- x,\bar{x},\bar{x}$ | (11) $3^- \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ | (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$ | (14) $2 x,\bar{x}+\frac{3}{4},\frac{1}{8}$ | (15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},-\frac{1}{4},z$ | (16) $4^+(0,0,\frac{1}{4})$ $0,\frac{1}{4},z$ |
| (17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$ | (18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,y$ | (19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$ | (20) $4^+(\frac{3}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$ |
| (21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$ | (22) $2(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},x$ | (23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ | (24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$ |
| (25) $\bar{1} \frac{3}{8},\frac{3}{8},\frac{1}{8}$ | (26) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{3}{8}$ | (27) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$ | (28) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,z$ |
| (29) $\bar{3}^+ x+\frac{1}{2},x,x$; $\frac{5}{8},\frac{1}{8},\frac{1}{8}$ | (30) $\bar{3}^+ \bar{x}-\frac{3}{2},x+1,\bar{x}$; $-\frac{5}{8},\frac{1}{8},\frac{7}{8}$ | (31) $\bar{3}^+ x+\frac{1}{2},\bar{x}+1,\bar{x}$; $\frac{5}{8},\frac{7}{8},-\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x}+\frac{1}{2},\bar{x},x$; $\frac{3}{8},-\frac{1}{8},\frac{1}{8}$ |
| (33) $\bar{3}^- x,x+\frac{1}{2},x$; $\frac{1}{8},\frac{5}{8},\frac{1}{8}$ | (34) $\bar{3}^- x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{8},-\frac{1}{8},\frac{3}{8}$ | (35) $\bar{3}^- \bar{x}-\frac{1}{2},\bar{x}+1,x$; $-\frac{5}{8},\frac{7}{8},\frac{1}{8}$ | (36) $\bar{3}^- \bar{x}+1,x,\bar{x}$; $\frac{7}{8},\frac{1}{8},-\frac{1}{8}$ |
| (37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$ | (38) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z | (39) $\bar{4}^- \frac{1}{4},\frac{1}{4},z; \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (40) $\bar{4}^+ 0,0,z; 0,0,0$ |
| (41) $\bar{4}^- x,0,\frac{1}{2}; 0,0,\frac{1}{2}$ | (42) $m x,y,\bar{y}$ | (43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$ | (44) $\bar{4}^+ x,\frac{1}{4},\frac{1}{4}; \frac{1}{4},\frac{1}{4},\frac{1}{4}$ |
| (45) $\bar{4}^+ -\frac{1}{4},y,\frac{1}{4}; -\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (46) $m \bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^- 0,y,0; 0,0,0$ | (48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x+\frac{1}{4},y,x$ |

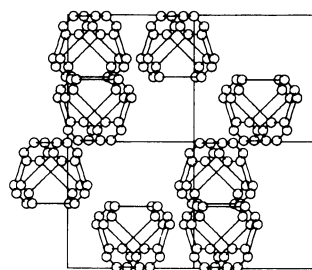
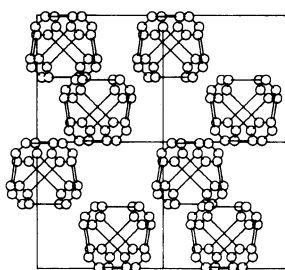
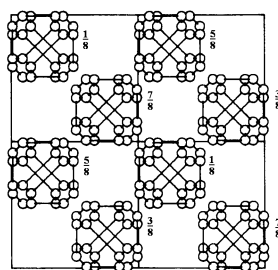
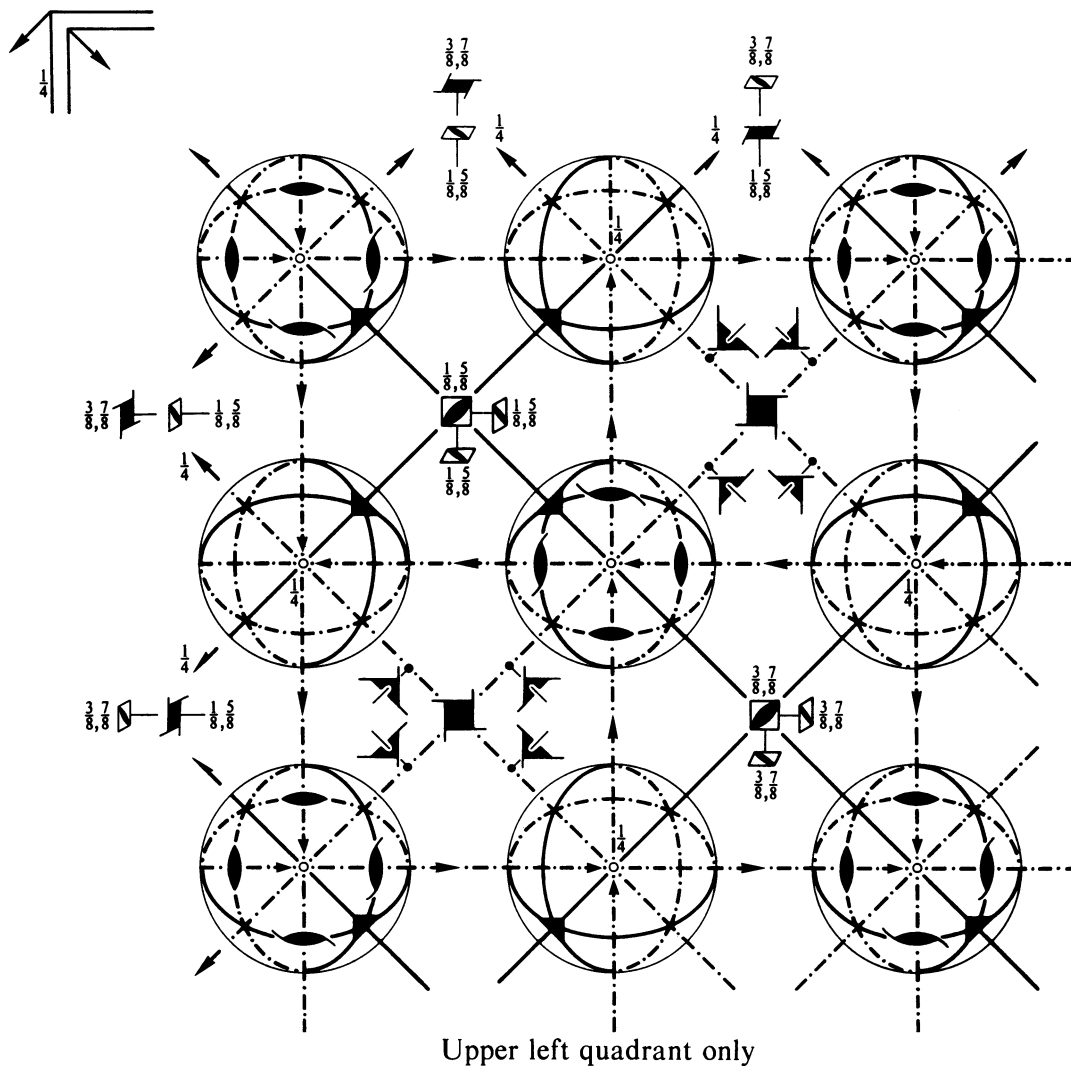
$F d \bar{3} m$ O_h^7 $m \bar{3} m$

Cubic

No. 227

 $F 4_1/d \bar{3} 2/m$ Patterson symmetry $F m \bar{3} m$

ORIGIN CHOICE 2



Origin at centre ($\bar{3}m$), at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from $\bar{4}3m$

Asymmetric unit $-\frac{1}{8} \leq x \leq \frac{3}{8}; -\frac{1}{8} \leq y \leq 0; -\frac{1}{4} \leq z \leq 0; y \leq \min(\frac{1}{4} - x, x); -y - \frac{1}{4} \leq z \leq y$
Vertices $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{3}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{1}{4}, 0, 0; 0, 0, 0; \frac{1}{4}, 0, -\frac{1}{4}; 0, 0, -\frac{1}{4}$

Symmetry operations

(given on page 703)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	h, k, l permutable General:

192	i	1	(1) x, y, z	(2) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{4}, y + \frac{1}{2}, \bar{z} + \frac{3}{4}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$	$hkl : h + k = 2n$ and $h + l, k + l = 2n$
			(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{y} + \frac{1}{4}$	(7) $\bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{1}{4}, x + \frac{1}{2}, \bar{y} + \frac{3}{4}$	$OkL : k + l = 4n$ and $k, l = 2n$
			(9) y, z, x	(10) $\bar{y} + \frac{1}{4}, z + \frac{1}{2}, \bar{x} + \frac{3}{4}$	(11) $y + \frac{1}{2}, \bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}$	(12) $\bar{y} + \frac{3}{4}, \bar{z} + \frac{1}{4}, x + \frac{1}{2}$	$hhl : h + l = 2n$
			(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{2}$	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) $y + \frac{1}{4}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$	(16) $\bar{y} + \frac{1}{2}, x + \frac{3}{4}, z + \frac{1}{4}$	$h00 : h = 4n$
			(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{1}{2}$	(18) $\bar{x} + \frac{1}{2}, z + \frac{3}{4}, y + \frac{1}{4}$	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) $x + \frac{1}{4}, \bar{z} + \frac{1}{2}, y + \frac{3}{4}$	
			(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{1}{2}$	(22) $z + \frac{1}{4}, \bar{y} + \frac{1}{2}, x + \frac{3}{4}$	(23) $\bar{z} + \frac{1}{2}, y + \frac{3}{4}, x + \frac{1}{4}$	(24) $\bar{z}, \bar{y}, \bar{x}$	
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{1}{2}$	(27) $x + \frac{3}{4}, \bar{y} + \frac{1}{2}, z + \frac{1}{4}$	(28) $\bar{x} + \frac{1}{2}, y + \frac{1}{4}, z + \frac{3}{4}$	
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z} + \frac{1}{2}, x + \frac{1}{4}, y + \frac{3}{4}$	(31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{1}{2}$	(32) $z + \frac{3}{4}, \bar{x} + \frac{1}{2}, y + \frac{1}{4}$	
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y + \frac{3}{4}, \bar{z} + \frac{1}{2}, x + \frac{1}{4}$	(35) $\bar{y} + \frac{1}{2}, z + \frac{1}{4}, x + \frac{3}{4}$	(36) $y + \frac{1}{4}, z + \frac{3}{4}, \bar{x} + \frac{1}{2}$	
			(37) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{1}{2}$	(38) y, x, z	(39) $\bar{y} + \frac{3}{4}, x + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(40) $y + \frac{1}{2}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$	
			(41) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{1}{2}$	(42) $x + \frac{1}{2}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(43) x, z, y	(44) $\bar{x} + \frac{3}{4}, z + \frac{1}{2}, \bar{y} + \frac{1}{4}$	
			(45) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{1}{2}$	(46) $\bar{z} + \frac{3}{4}, y + \frac{1}{2}, \bar{x} + \frac{1}{4}$	(47) $z + \frac{1}{2}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(48) z, y, x	

Special: as above, plus

no extra conditions

96	h	..2	$0, y, \bar{y}$	$\frac{3}{4}, \bar{y} + \frac{1}{4}, \bar{y} + \frac{1}{2}$	$\frac{1}{4}, y + \frac{1}{2}, y + \frac{3}{4}$	$\frac{1}{2}, \bar{y} + \frac{3}{4}, y + \frac{1}{4}$
			$\bar{y}, 0, y$	$\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y} + \frac{1}{4}$	$y + \frac{3}{4}, \frac{1}{4}, y + \frac{1}{2}$	$y + \frac{1}{4}, \frac{1}{2}, \bar{y} + \frac{3}{4}$
			$y, \bar{y}, 0$	$\bar{y} + \frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{3}{4}$	$y + \frac{1}{2}, y + \frac{3}{4}, \frac{1}{4}$	$\bar{y} + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2}$
			$0, \bar{y}, y$	$\frac{1}{4}, y + \frac{3}{4}, y + \frac{1}{2}$	$\frac{3}{4}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}$	$\frac{1}{2}, y + \frac{1}{4}, \bar{y} + \frac{3}{4}$
			$y, 0, \bar{y}$	$y + \frac{1}{2}, \frac{1}{4}, y + \frac{3}{4}$	$\bar{y} + \frac{1}{4}, \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\bar{y} + \frac{3}{4}, \frac{1}{2}, y + \frac{1}{4}$
			$\bar{y}, \bar{y}, 0$	$y + \frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}, \frac{3}{4}$	$y + \frac{1}{4}, \bar{y} + \frac{3}{4}, \frac{1}{2}$

96	g	..m	x, x, z	$\bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{1}{2}$	$\bar{x} + \frac{1}{4}, x + \frac{1}{2}, \bar{z} + \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{z} + \frac{1}{4}$	no extra conditions
			z, x, x	$z + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}$	$\bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x + \frac{1}{2}$	$\bar{z} + \frac{1}{4}, x + \frac{1}{2}, \bar{x} + \frac{3}{4}$	
			x, z, x	$\bar{x} + \frac{1}{4}, z + \frac{1}{2}, \bar{x} + \frac{3}{4}$	$x + \frac{1}{2}, \bar{z} + \frac{3}{4}, \bar{x} + \frac{1}{4}$	$\bar{x} + \frac{3}{4}, \bar{z} + \frac{1}{4}, x + \frac{1}{2}$	
			$x + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\bar{x}, \bar{x}, \bar{z}$	$x + \frac{1}{4}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{3}{4}, z + \frac{1}{4}$	
			$x + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, z + \frac{3}{4}, x + \frac{1}{4}$	$\bar{x}, \bar{z}, \bar{x}$	$x + \frac{1}{4}, \bar{z} + \frac{1}{2}, x + \frac{3}{4}$	
			$z + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{2}$	$z + \frac{1}{4}, \bar{x} + \frac{1}{2}, x + \frac{3}{4}$	$\bar{z} + \frac{1}{2}, x + \frac{3}{4}, x + \frac{1}{4}$	$\bar{z}, \bar{x}, \bar{x}$	

48	f	2.mm	$x, \frac{1}{8}, \frac{1}{8}$	$\bar{x} + \frac{3}{4}, \frac{1}{8}, \frac{5}{8}$	$\frac{1}{8}, x, \frac{1}{8}$	$\frac{5}{8}, \bar{x} + \frac{3}{4}, \frac{1}{8}$	$\frac{1}{8}, \frac{1}{8}, x$	$\frac{1}{8}, \frac{5}{8}, \bar{x} + \frac{3}{4}$	$hkl : h = 2n + 1$ or $h + k + l = 4n$
			$\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}$	$\frac{7}{8}, \bar{x}, \frac{7}{8}$	$x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}$	$\bar{x} + \frac{1}{2}, \frac{7}{8}, \frac{3}{8}$	$\frac{7}{8}, \frac{3}{8}, \bar{x} + \frac{1}{2}$	$\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}$	

32	e	.3m	x, x, x	$\bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x + \frac{1}{2}$				no extra conditions
			$\bar{x} + \frac{1}{4}, x + \frac{1}{2}, \bar{x} + \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}$				
			$x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{x}, \bar{x}$				
			$x + \frac{1}{4}, \bar{x} + \frac{1}{2}, x + \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{3}{4}, x + \frac{1}{4}$				

16	d	. $\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{1}{4}$	$0, \frac{1}{4}, \frac{3}{4}$	} $hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$
16	c	. $\bar{3}m$	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	

8	b	$\bar{4}3m$	$\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{5}{8}, \frac{1}{8}$	} $hkl : h = 2n + 1$ or $h + k + l = 4n$
8	a	$\bar{4}3m$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{3}{8}$	

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{8}, \frac{3}{8}, z$ Along [111] $p6mm$

$$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x Along [110] $c2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

ORIGIN CHOICE 2

Maximal non-isomorphic subgroups

I	[2] $F \bar{4} 3 m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F 4_1 3 2$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $F d \bar{3} 1$ ($F d \bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	{ [3] $F 4_1/d 1 2/m$ ($I 4_1/am d$, 141)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	{ [3] $F 4_1/d 1 2/m$ ($I 4_1/am d$, 141)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	{ [3] $F 4_1/d 1 2/m$ ($I 4_1/am d$, 141)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	{ [4] $F 1 \bar{3} 2/m$ ($R \bar{3} m$, 166)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F d \bar{3} m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (227)

Minimal non-isomorphic supergroups

I none

II [2] $P n \bar{3} m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---|--|--|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \frac{3}{8}, \frac{3}{8}, z$ | (3) $2(0,\frac{1}{2},0) \frac{1}{8}, y, \frac{3}{8}$ | (4) $2(\frac{1}{2},0,0) x, \frac{3}{8}, \frac{3}{8}$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x + \frac{1}{4}, \bar{x}$ | (7) $3^+ x + \frac{3}{4}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{5}{12}, \bar{x} + \frac{1}{6}, \bar{x}$ | (11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \bar{x} + \frac{7}{12}, \bar{x} + \frac{5}{12}, x$ | (12) $3^- (\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \bar{x} - \frac{1}{6}, x + \frac{7}{12}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{4}, \frac{1}{4}$ | (14) $2 x, \bar{x}, 0$ | (15) $4^-(0,0,\frac{3}{4}) \frac{3}{8}, \frac{1}{8}, z$ | (16) $4^+(0,0,\frac{1}{4}) -\frac{1}{8}, \frac{5}{8}, z$ |
| (17) $4^-(\frac{3}{4},0,0) x, \frac{3}{8}, \frac{3}{8}$ | (18) $2(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4}, y + \frac{1}{4}, y$ | (19) $2 0, y, \bar{y}$ | (20) $4^+(\frac{1}{4},0,0) x, -\frac{1}{8}, \frac{5}{8}$ |
| (21) $4^+(0,\frac{1}{4},0) \frac{5}{8}, y, -\frac{1}{8}$ | (22) $2(\frac{1}{2},0,\frac{1}{2}) x - \frac{1}{4}, \frac{1}{4}, x$ | (23) $4^-(0,\frac{3}{4},0) \frac{1}{8}, y, \frac{3}{8}$ | (24) $2 \bar{x}, 0, x$ |
| (25) $\bar{1} 0, 0, 0$ | (26) $d(\frac{1}{4}, \frac{3}{4}, 0) x, y, \frac{1}{4}$ | (27) $d(\frac{3}{4}, 0, \frac{1}{4}) x, \frac{1}{4}, z$ | (28) $d(0, \frac{1}{4}, \frac{3}{4}) \frac{1}{4}, y, z$ |
| (29) $\bar{3}^+ x, x, x; 0, 0, 0$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{3}{4}, \bar{x}; -\frac{1}{4}, 0, \frac{3}{4}$ | (31) $\bar{3}^+ x - \frac{1}{4}, \bar{x} + 1, \bar{x}; 0, \frac{3}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} - \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, 0$ |
| (33) $\bar{3}^- x, x, x; 0, 0, 0$ | (34) $\bar{3}^- x + \frac{5}{4}, \bar{x} - 1, \bar{x}; \frac{1}{2}, -\frac{1}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{5}{4}, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ | (36) $\bar{3}^- \bar{x} + 1, x + \frac{1}{4}, \bar{x}; \frac{3}{4}, \frac{1}{2}, -\frac{1}{4}$ |
| (37) $g(-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$ | (38) $m x, x, z$ | (39) $\bar{4}^- \frac{1}{8}, \frac{5}{8}, z; \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ | (40) $\bar{4}^+ \frac{3}{8}, -\frac{1}{8}, z; \frac{3}{8}, -\frac{1}{8}, \frac{3}{8}$ |
| (41) $\bar{4}^- x, \frac{1}{8}, \frac{5}{8}; \frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (42) $g(\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}) x, y + \frac{1}{2}, \bar{y}$ | (43) $m x, y, y$ | (44) $\bar{4}^+ x, \frac{3}{8}, -\frac{1}{8}; \frac{3}{8}, \frac{3}{8}, -\frac{1}{8}$ |
| (45) $\bar{4}^+ -\frac{1}{8}, y, \frac{3}{8}; -\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$ | (46) $g(\frac{1}{4}, \frac{1}{2}, -\frac{1}{4}) \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{5}{8}, y, \frac{1}{8}; \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ | (48) $m x, y, x$ |

For (0,1/2,1/2)+ set

- | | | | |
|--|--|--|--|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) $2 \frac{3}{8}, \frac{3}{8}, z$ | (3) $2 \frac{1}{8}, y, \frac{1}{8}$ | (4) $2(\frac{1}{2},0,0) x, \frac{1}{8}, \frac{3}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{3}, x - \frac{1}{6}, x$ | (6) $3^+(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}) \bar{x} + \frac{1}{6}, x + \frac{5}{12}, \bar{x}$ | (7) $3^+ x + \frac{3}{4}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{6}, x + \frac{1}{6}, x$ | (10) $3^- x + \frac{1}{4}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x$ | (12) $3^- \bar{x}, x + \frac{3}{4}, \bar{x}$ |
| (13) $2(\frac{3}{4}, \frac{1}{4}, 0) x, x, 0$ | (14) $2(-\frac{1}{4}, \frac{1}{4}, 0) x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ | (15) $4^-(0,0,\frac{1}{4}) \frac{1}{8}, -\frac{1}{8}, z$ | (16) $4^+(0,0,\frac{3}{4}) \frac{1}{8}, \frac{3}{8}, z$ |
| (17) $4^-(\frac{3}{4},0,0) x, \frac{3}{8}, -\frac{3}{8}$ | (18) $2(0,\frac{1}{2},\frac{1}{2}) \frac{1}{4}, y - \frac{1}{4}, y$ | (19) $2 0, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{4},0,0) x, -\frac{1}{8}, \frac{1}{8}$ |
| (21) $4^+(0,\frac{3}{4},0) \frac{3}{8}, y, -\frac{3}{8}$ | (22) $2(\frac{1}{4},0,\frac{1}{4}) x, 0, x$ | (23) $4^-(0,\frac{1}{4},0) -\frac{1}{8}, y, \frac{5}{8}$ | (24) $2(-\frac{1}{4},0,\frac{1}{4}) \bar{x} + \frac{1}{4}, \frac{1}{4}, x$ |
| (25) $\bar{1} 0, \frac{1}{4}, \frac{1}{4}$ | (26) $d(\frac{1}{4}, \frac{1}{4}, 0) x, y, 0$ | (27) $d(\frac{3}{4}, 0, \frac{3}{4}) x, 0, z$ | (28) $d(0, \frac{3}{4}, \frac{1}{4}) \frac{1}{4}, y, z$ |
| (29) $\bar{3}^+ x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{5}{4}, \bar{x}; -\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ | (31) $\bar{3}^+ x - \frac{1}{4}, \bar{x} + \frac{1}{2}, \bar{x}; 0, \frac{1}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} - \frac{3}{4}, x; \frac{3}{4}, -\frac{3}{4}, 0$ |
| (33) $\bar{3}^- x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (34) $\bar{3}^- x + \frac{3}{4}, \bar{x} - \frac{3}{2}, \bar{x}; 0, -\frac{3}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{4}, \bar{x} + \frac{3}{4}, x; -\frac{1}{4}, \frac{3}{4}, 0$ | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, x - \frac{1}{4}, \bar{x}; \frac{1}{4}, 0, -\frac{1}{4}$ |
| (37) $m x + \frac{1}{4}, \bar{x}, z$ | (38) $g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) x - \frac{1}{4}, x, z$ | (39) $\bar{4}^- \frac{3}{8}, \frac{5}{8}, z; \frac{3}{8}, \frac{5}{8}, \frac{3}{8}$ | (40) $\bar{4}^+ \frac{5}{8}, \frac{3}{8}, z; \frac{5}{8}, \frac{1}{8}, \frac{1}{8}$ |
| (41) $\bar{4}^- x, \frac{1}{8}, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (42) $g(\frac{1}{2}, \frac{1}{4}, -\frac{1}{4}) x, y + \frac{1}{2}, \bar{y}$ | (43) $g(0, \frac{1}{2}, \frac{1}{2}) x, y, y$ | (44) $\bar{4}^+ x, \frac{3}{8}, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ |
| (45) $\bar{4}^+ \frac{1}{8}, y, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (46) $m \bar{x} + \frac{3}{4}, y, x$ | (47) $\bar{4}^- \frac{3}{8}, y, -\frac{1}{8}; \frac{3}{8}, \frac{3}{8}, -\frac{1}{8}$ | (48) $g(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) x - \frac{1}{4}, y, x$ |

For (1/2,0,1/2)+ set

- | | | | |
|--|--|--|--|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) $2 \frac{1}{8}, \frac{1}{8}, z$ | (3) $2(0,\frac{1}{2},0) \frac{3}{8}, y, \frac{1}{8}$ | (4) $2 x, \frac{3}{8}, \frac{3}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x - \frac{1}{6}, x$ | (6) $3^+ \bar{x}, x + \frac{3}{4}, \bar{x}$ | (7) $3^+ x + \frac{1}{4}, \bar{x}, \bar{x}$ | (8) $3^+(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}) \bar{x} + \frac{5}{12}, \bar{x} + \frac{7}{12}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x - \frac{1}{6}, x - \frac{1}{3}, x$ | (10) $3^- x + \frac{1}{4}, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ | (12) $3^- \bar{x}, x + \frac{1}{4}, \bar{x}$ |
| (13) $2(\frac{1}{4}, \frac{1}{4}, 0) x, x, 0$ | (14) $2(\frac{1}{4}, -\frac{1}{4}, 0) x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ | (15) $4^-(0,0,\frac{1}{4}) \frac{5}{8}, -\frac{1}{8}, z$ | (16) $4^+(0,0,\frac{3}{4}) -\frac{3}{8}, \frac{3}{8}, z$ |
| (17) $4^-(\frac{1}{4},0,0) x, \frac{1}{8}, -\frac{1}{8}$ | (18) $2(0,\frac{3}{4},\frac{3}{4}) 0, y, y$ | (19) $2(0,-\frac{1}{4},\frac{1}{4}) \frac{1}{4}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{3}{4},0,0) x, \frac{1}{8}, \frac{3}{8}$ |
| (21) $4^+(0,\frac{1}{4},0) \frac{1}{8}, y, -\frac{1}{8}$ | (22) $2(\frac{1}{2},0,\frac{1}{2}) x + \frac{1}{4}, \frac{1}{4}, x$ | (23) $4^-(0,\frac{3}{4},0) -\frac{3}{8}, y, \frac{3}{8}$ | (24) $2 \bar{x} + \frac{1}{2}, 0, x$ |
| (25) $\bar{1} \frac{1}{4}, 0, \frac{1}{4}$ | (26) $d(\frac{3}{4}, \frac{3}{4}, 0) x, y, 0$ | (27) $d(\frac{1}{4}, 0, \frac{3}{4}) x, \frac{1}{4}, z$ | (28) $d(0, \frac{1}{4}, \frac{1}{4}) 0, y, z$ |
| (29) $\bar{3}^+ x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{4}, \bar{x}; -\frac{1}{4}, 0, \frac{1}{4}$ | (31) $\bar{3}^+ x - \frac{3}{4}, \bar{x} + \frac{3}{2}, \bar{x}; 0, \frac{3}{4}, -\frac{3}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{3}{4}, \bar{x} + \frac{1}{4}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{2}$ |
| (33) $\bar{3}^- x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (34) $\bar{3}^- x + \frac{3}{4}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{4}, x; -\frac{1}{4}, \frac{1}{4}, 0$ | (36) $\bar{3}^- \bar{x} + \frac{3}{2}, x - \frac{3}{4}, \bar{x}; \frac{3}{4}, 0, -\frac{3}{4}$ |
| (37) $m x + \frac{3}{4}, \bar{x}, z$ | (38) $g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) x + \frac{1}{4}, x, z$ | (39) $\bar{4}^- -\frac{1}{8}, \frac{3}{8}, z; -\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$ | (40) $\bar{4}^+ \frac{1}{8}, \frac{1}{8}, z; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ |
| (41) $\bar{4}^- x, \frac{3}{8}, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (42) $m x, y + \frac{1}{4}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}) x, y - \frac{1}{4}, y$ | (44) $\bar{4}^+ x, \frac{5}{8}, \frac{1}{8}; \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ |
| (45) $\bar{4}^+ \frac{3}{8}, y, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (46) $g(-\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{8}, y, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (48) $g(\frac{1}{2}, 0, \frac{1}{2}) x, y, x$ |

For (1/2,1/2,0)+ set

- | | | | |
|---|--|---|--|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2}) \frac{1}{8}, \frac{3}{8}, z$ | (3) $2 \frac{3}{8}, y, \frac{3}{8}$ | (4) $2 x, \frac{1}{8}, \frac{1}{8}$ |
| (5) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{6}, x + \frac{1}{3}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{4}, \bar{x}$ | (7) $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{7}{12}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{3}{4}, \bar{x} + \frac{3}{4}, x$ |
| (9) $3^-(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{3}, x + \frac{1}{6}, x$ | (10) $3^- x + \frac{3}{4}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{3}{4}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{4}, \frac{1}{4}$ | (14) $2 x, \bar{x} + \frac{1}{2}, 0$ | (15) $4^-(0,0,\frac{3}{4}) \frac{3}{8}, -\frac{3}{8}, z$ | (16) $4^+(0,0,\frac{1}{4}) -\frac{1}{8}, \frac{1}{8}, z$ |
| (17) $4^-(\frac{1}{4},0,0) x, \frac{5}{8}, -\frac{1}{8}$ | (18) $2(0,\frac{1}{4},\frac{1}{4}) 0, y, y$ | (19) $2(0,\frac{1}{4}, -\frac{1}{4}) \frac{1}{4}, y + \frac{1}{4}, \bar{y}$ | (20) $4^+(\frac{3}{4},0,0) x, -\frac{3}{8}, \frac{3}{8}$ |
| (21) $4^+(0,\frac{3}{4},0) \frac{3}{8}, y, \frac{1}{8}$ | (22) $2(\frac{3}{4},0,\frac{3}{4}) x, 0, x$ | (23) $4^-(0,\frac{1}{4},0) -\frac{1}{8}, y, \frac{1}{8}$ | (24) $2(\frac{1}{4},0, -\frac{1}{4}) \bar{x} + \frac{1}{4}, \frac{1}{4}, x$ |
| (25) $\bar{1} \frac{1}{4}, \frac{1}{4}, 0$ | (26) $d(\frac{3}{4}, \frac{1}{4}, 0) x, y, \frac{1}{4}$ | (27) $d(\frac{1}{4}, 0, \frac{1}{4}) x, 0, z$ | (28) $d(0, \frac{3}{4}, \frac{3}{4}) 0, y, z$ |
| (29) $\bar{3}^+ x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (30) $\bar{3}^+ \bar{x} - \frac{3}{2}, x + \frac{3}{4}, \bar{x}; -\frac{3}{4}, 0, \frac{3}{4}$ | (31) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + 1, \bar{x}; \frac{1}{2}, \frac{3}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{4}, \bar{x} - \frac{1}{4}, x; \frac{1}{4}, -\frac{1}{4}, 0$ |
| (33) $\bar{3}^- x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (34) $\bar{3}^- x + \frac{1}{4}, \bar{x} - \frac{1}{2}, \bar{x}; 0, -\frac{1}{4}, \frac{1}{4}$ | (35) $\bar{3}^- \bar{x} - \frac{3}{4}, \bar{x} + \frac{3}{4}, x; -\frac{3}{4}, \frac{3}{4}, 0$ | (36) $\bar{3}^- \bar{x} + 1, x - \frac{1}{4}, \bar{x}; \frac{3}{4}, 0, -\frac{1}{4}$ |
| (37) $g(\frac{1}{4}, -\frac{1}{4}, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, 0) x, x, z$ | (39) $\bar{4}^- \frac{1}{8}, \frac{1}{8}, z; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (40) $\bar{4}^+ \frac{3}{8}, \frac{3}{8}, z; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ |
| (41) $\bar{4}^- x, -\frac{1}{8}, \frac{3}{8}; \frac{3}{8}, -\frac{1}{8}, \frac{3}{8}$ | (42) $m x, y + \frac{3}{4}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}) x, y + \frac{1}{4}, y$ | (44) $\bar{4}^+ x, \frac{1}{8}, \frac{1}{8}; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ |
| (45) $\bar{4}^+ \frac{1}{8}, y, \frac{3}{8}; \frac{1}{8}, \frac{1}{8}, \frac{5}{8}$ | (46) $m \bar{x} + \frac{1}{4}, y, x$ | (47) $\bar{4}^- \frac{3}{8}, y, \frac{3}{8}; \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$ | (48) $g(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}) x + \frac{1}{4}, y, x$ |

$Fd\bar{3}c$

O_h^8

$m\bar{3}m$

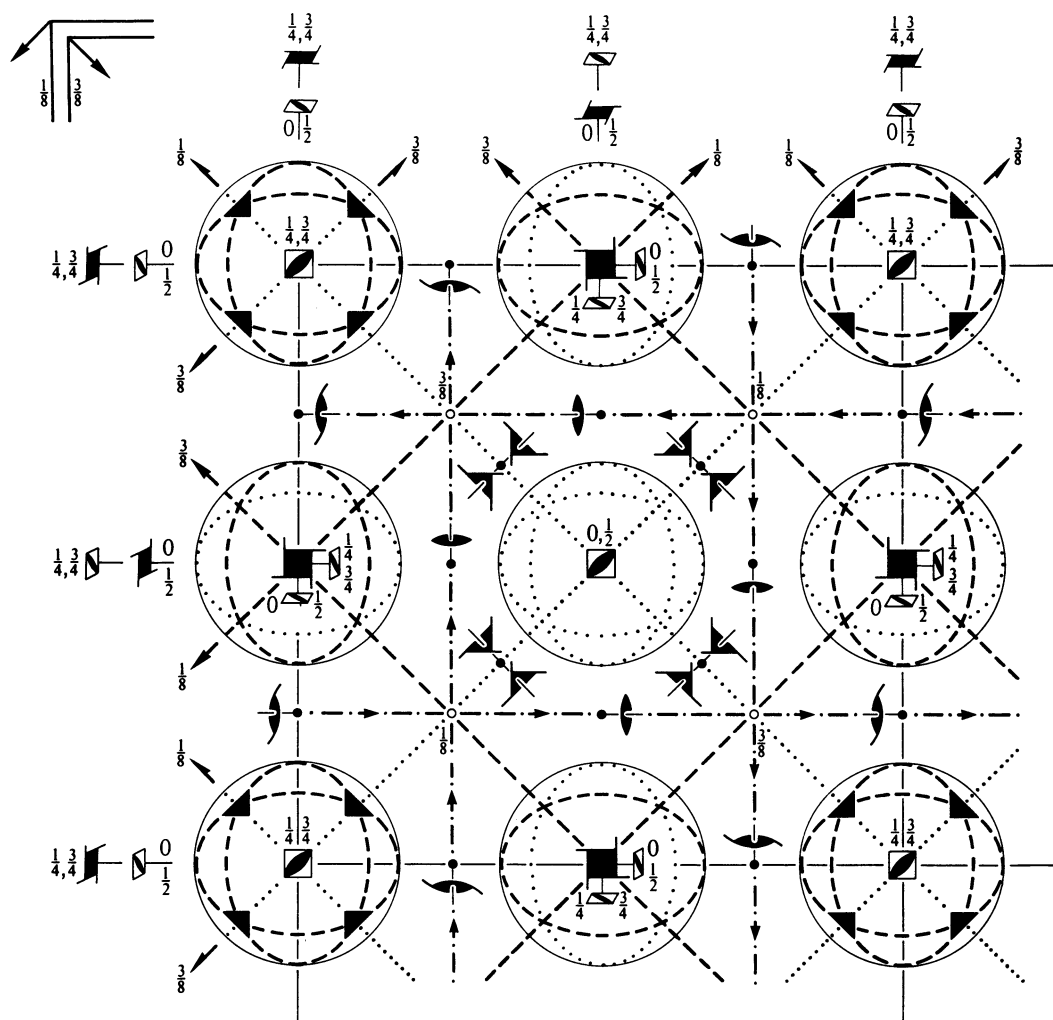
Cubic

No. 228

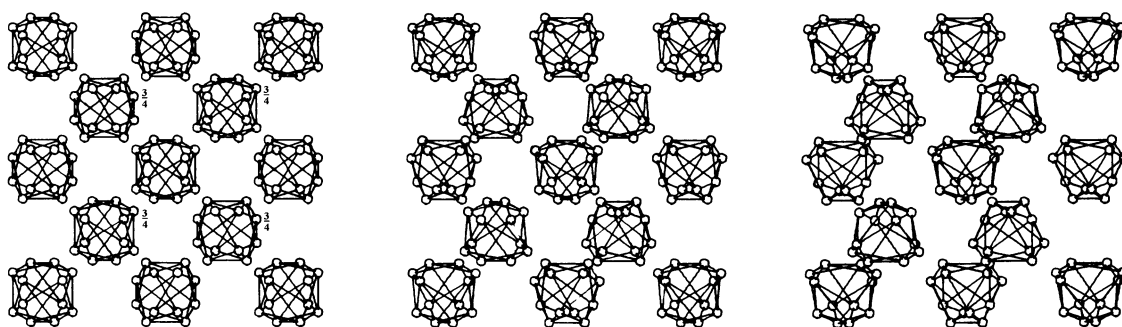
$F 4_1/d \bar{3} 2/c$

Patterson symmetry $Fm\bar{3}m$

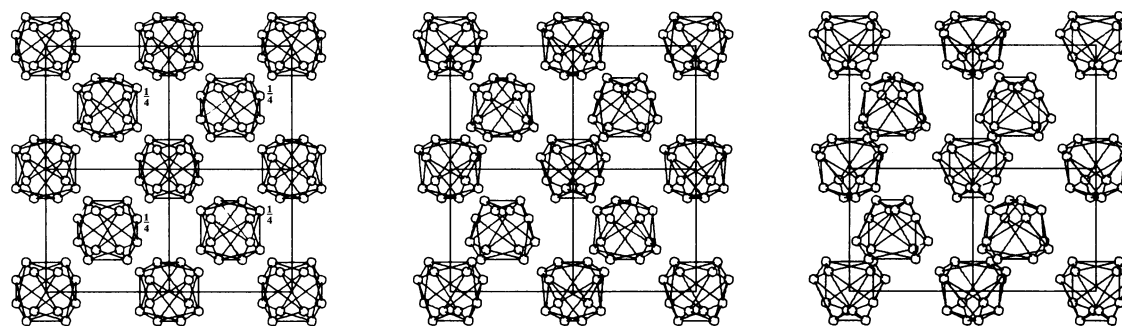
ORIGIN CHOICE 1



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Origin at 23, at $-\frac{3}{8}, -\frac{3}{8}, -\frac{3}{8}$ from centre ($\bar{3}$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{8}; -\frac{1}{8} \leq z \leq \frac{1}{8}; y \leq \min(\frac{1}{2} - x, x); -y \leq z \leq y$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{3}{8}, \frac{1}{8}, \frac{1}{8} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8} \quad \frac{3}{8}, \frac{1}{8}, -\frac{1}{8} \quad \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$

Symmetry operations

(given on page 707)

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity,		Coordinates		Reflection conditions
Wyckoff letter,				
Site symmetry		$(0, 0, 0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$
		$(\frac{1}{2}, \frac{1}{2}, 0)+$		

h, k, l permutable
General:

192	h	1	(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$	$hkl : h + k = 2n$ and $h + l, k + l = 2n$ $0kl : k + l = 4n$ and $k, l = 2n$ $hhl : h, l = 2n$ $h00 : h = 4n$
			(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$	(7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	
			(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	(11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	(12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	
			(13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$	(14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$	(16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	
			(17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$	(18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$	(19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$	
			(21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$	(23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$	(24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	
			(25) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(26) $x + \frac{3}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(27) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{3}{4}$	(28) $\bar{x} + \frac{1}{4}, y + \frac{3}{4}, z + \frac{1}{4}$	
			(29) $\bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}$	(30) $\bar{z} + \frac{1}{4}, x + \frac{3}{4}, y + \frac{1}{4}$	(31) $z + \frac{3}{4}, x + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(32) $z + \frac{1}{4}, \bar{x} + \frac{1}{4}, y + \frac{3}{4}$	
			(33) $\bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}$	(34) $y + \frac{1}{4}, \bar{z} + \frac{1}{4}, x + \frac{3}{4}$	(35) $\bar{y} + \frac{1}{4}, z + \frac{3}{4}, x + \frac{1}{4}$	(36) $y + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{4}$	
			(37) $\bar{y}, \bar{x} + \frac{1}{2}, z$	(38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(39) $\bar{y} + \frac{1}{2}, x, \bar{z}$	(40) $y, \bar{x}, \bar{z} + \frac{1}{2}$	
			(41) $\bar{x}, \bar{z} + \frac{1}{2}, y$	(42) $x, \bar{z}, \bar{y} + \frac{1}{2}$	(43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(44) $\bar{x} + \frac{1}{2}, z, \bar{y}$	
			(45) $\bar{z}, \bar{y} + \frac{1}{2}, x$	(46) $\bar{z} + \frac{1}{2}, y, \bar{x}$	(47) $z, \bar{y}, \bar{x} + \frac{1}{2}$	(48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	

Special: as above, plus

no extra conditions

$hkl : h + k + l = 4n$

$hkl : h = 2n$

$hkl : h + k + l = 4n$

$hkl : h, k, l = 4n + 2$
or $h, k, l = 4n$

$hkl : h, k, l = 4n + 2$
or $h, k, l = 4n$

$hkl : h + k + l = 4n$

ORIGIN CHOICE 1

Symmetry of special projections

Along $[001] p4mm$

$$\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$

Along $[111] p6mm$

$$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110] p2mm$

$$\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, \frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	{ [3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	{ [3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	{ [3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (228)

Minimal non-isomorphic supergroups

I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ | (4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$ |
| (5) $3^+ x,x,x$ | (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ | (7) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ |
| (9) $3^- x,x,x$ | (10) $3^- x,\bar{x}+\frac{1}{2},\bar{x}$ | (11) $3^- \bar{x}+\frac{1}{2},\bar{x},x$ | (12) $3^- \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$ | (14) $2 x,\bar{x}+\frac{1}{4},\frac{1}{8}$ | (15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},\frac{1}{4},z$ | (16) $4^+(0,0,\frac{1}{4})$ $0,\frac{3}{4},z$ |
| (17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},\frac{1}{4}$ | (18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y+\frac{1}{4},y$ | (19) $2 \frac{1}{8},y+\frac{1}{4},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{3}{4}$ |
| (21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{4},y,0$ | (22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{3}{8},x$ | (23) $4^-(0,\frac{3}{4},0)$ $\frac{1}{4},y,\frac{1}{2}$ | (24) $2 \bar{x}+\frac{1}{4},\frac{1}{8},x$ |
| (25) $\bar{1} \frac{3}{8},\frac{3}{8},\frac{3}{8}$ | (26) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{1}{8}$ | (27) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$ | (28) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{1}{8},y,z$ |
| (29) $\bar{3}^+ x,x,x,x;$ $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ | (30) $\bar{3}^+ \bar{x}-1,x+1,\bar{x};$ $-\frac{3}{8},\frac{3}{8},\frac{3}{8}$ | (31) $\bar{3}^+ x,\bar{x}+1,\bar{x};$ $\frac{3}{8},\frac{5}{8},-\frac{3}{8}$ | (32) $\bar{3}^+ \bar{x}+1,\bar{x},x;$ $\frac{5}{8},-\frac{3}{8},\frac{3}{8}$ |
| (33) $\bar{3}^- x,x,x,x;$ $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ | (34) $\bar{3}^- x+\frac{1}{2},\bar{x}-1,\bar{x};$ $-\frac{1}{8},-\frac{3}{8},\frac{5}{8}$ | (35) $\bar{3}^- \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;$ $-\frac{3}{8},\frac{5}{8},-\frac{1}{8}$ | (36) $\bar{3}^- \bar{x}+1,x-\frac{1}{2},\bar{x};$ $\frac{5}{8},-\frac{1}{8},-\frac{3}{8}$ |
| (37) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$ | (38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z | (39) $\bar{4}^- \frac{1}{4},\frac{1}{4},z;$ $\frac{1}{4},\frac{1}{4},0$ | (40) $\bar{4}^+ 0,0,z;$ $0,0,\frac{1}{4}$ |
| (41) $\bar{4}^- x,\frac{1}{4},\frac{1}{4};$ $0,\frac{1}{4},\frac{1}{4}$ | (42) $g(0,-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$ | (43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y | (44) $\bar{4}^+ x,0,0;$ $\frac{1}{4},0,0$ |
| (45) $\bar{4}^+ 0,y,0;$ $0,\frac{1}{4},0$ | (46) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^- \frac{1}{4},y,\frac{1}{4};$ $\frac{1}{4},0,\frac{1}{4}$ | (48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x |

For (0, $\frac{1}{2},\frac{1}{2}$)+ set

- | | | | |
|--|---|---|---|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) 2 0,0,z | (3) 2 $\frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$ | (6) $3^+ \bar{x}+\frac{1}{2},x,\bar{x}$ | (7) $3^+ x,\bar{x},\bar{x}$ | (8) $3^+ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$ | (10) $3^- x+\frac{1}{2},\bar{x},\bar{x}$ | (11) $3^-(\frac{1}{3},-\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^- \bar{x},x,\bar{x}$ |
| (13) $2(\frac{3}{4},\frac{3}{4},0)$ $x,x,\frac{1}{8}$ | (14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$ | (15) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},0,z$ | (16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$ |
| (17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},-\frac{1}{4}$ | (18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$ | (19) $2 \frac{1}{8},y+\frac{3}{4},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{1}{4}$ |
| (21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$ | (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},x$ | (23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$ | (24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$ |
| (25) $\bar{1} \frac{3}{8},\frac{1}{8},\frac{1}{8}$ | (26) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,\frac{3}{8}$ | (27) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$ | (28) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{1}{8},y,z$ |
| (29) $\bar{3}^+ x,x-\frac{1}{2},x;$ $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$ | (30) $\bar{3}^+ \bar{x}-1,x+\frac{1}{2},\bar{x};$ $-\frac{3}{8},-\frac{1}{8},\frac{5}{8}$ | (31) $\bar{3}^+ x,\bar{x}+\frac{3}{2},\bar{x};$ $\frac{3}{8},\frac{9}{8},-\frac{3}{8}$ | (32) $\bar{3}^+ \bar{x}+1,\bar{x}+\frac{1}{2},x;$ $\frac{5}{8},\frac{3}{8},\frac{3}{8}$ |
| (33) $\bar{3}^- x+\frac{1}{2},x+\frac{1}{2},x;$ $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$ | (34) $\bar{3}^- x+1,\bar{x}-\frac{1}{2},\bar{x};$ $\frac{3}{8},\frac{5}{8},\frac{3}{8}$ | (35) $\bar{3}^- \bar{x},\bar{x}+1,x;$ $-\frac{3}{8},\frac{5}{8},\frac{3}{8}$ | (36) $\bar{3}^- \bar{x}+\frac{3}{2},x,\bar{x};$ $\frac{9}{8},\frac{3}{8},-\frac{3}{8}$ |
| (37) $c x,\bar{x},z$ | (38) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$ | (39) $\bar{4}^- 0,\frac{1}{2},z;$ $0,\frac{1}{2},\frac{1}{4}$ | (40) $\bar{4}^+ \frac{1}{4},\frac{1}{4},z;$ $\frac{1}{4},\frac{1}{4},0$ |
| (41) $\bar{4}^- x,-\frac{1}{4},\frac{1}{4};$ $0,-\frac{1}{4},\frac{1}{4}$ | (42) $g(0,\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$ | (43) $a x,y,y$ | (44) $\bar{4}^+ x,\frac{1}{2},0;$ $\frac{1}{4},\frac{1}{2},0$ |
| (45) $\bar{4}^+ -\frac{1}{4},y,\frac{1}{4};$ $-\frac{1}{4},0,\frac{1}{4}$ | (46) $b \bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^- 0,y,0;$ $0,\frac{1}{4},0$ | (48) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$ |

For ($\frac{1}{2},0,\frac{1}{2}$)+ set

- | | | | |
|--|--|---|---|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ | (4) 2 $x,0,0$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$ | (6) $3^+ \bar{x},x,\bar{x}$ | (7) $3^+ x+\frac{1}{2},\bar{x},\bar{x}$ | (8) $3^+ \bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$ | (10) $3^-(\frac{1}{3},-\frac{1}{3},-\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^- \bar{x},\bar{x},x$ | (12) $3^- \bar{x},x+\frac{1}{2},\bar{x}$ |
| (13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,\frac{1}{8}$ | (14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$ | (15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$ | (16) $4^+(0,0,\frac{3}{4})$ $-\frac{1}{4},\frac{1}{2},z$ |
| (17) $4^-(\frac{1}{4},0,0)$ $x,\frac{1}{4},0$ | (18) $2(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,y$ | (19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$ | (20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$ |
| (21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{4},y,0$ | (22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$ | (23) $4^-(0,\frac{3}{4},0)$ $-\frac{1}{4},y,\frac{1}{2}$ | (24) $2 \bar{x}+\frac{3}{4},\frac{1}{8},x$ |
| (25) $\bar{1} \frac{1}{8},\frac{3}{8},\frac{1}{8}$ | (26) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,\frac{3}{8}$ | (27) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$ | (28) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{3}{8},y,z$ |
| (29) $\bar{3}^+ x+\frac{1}{2},x+\frac{1}{2},x;$ $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$ | (30) $\bar{3}^+ \bar{x}-\frac{3}{2},x+\frac{3}{2},\bar{x};$ $-\frac{3}{8},\frac{3}{8},\frac{9}{8}$ | (31) $\bar{3}^+ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};$ $\frac{3}{8},\frac{5}{8},\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;$ $\frac{5}{8},-\frac{3}{8},-\frac{1}{8}$ |
| (33) $\bar{3}^- x-\frac{1}{2},x,x;$ $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$ | (34) $\bar{3}^- x+1,\bar{x}-1,\bar{x};$ $\frac{3}{8},-\frac{3}{8},\frac{3}{8}$ | (35) $\bar{3}^- \bar{x},\bar{x}+\frac{3}{2},x;$ $-\frac{3}{8},\frac{9}{8},\frac{3}{8}$ | (36) $\bar{3}^- \bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x};$ $\frac{3}{8},\frac{3}{8},\frac{1}{8}$ |
| (37) $c x+\frac{1}{2},\bar{x},z$ | (38) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$ | (39) $\bar{4}^- 0,0,z;$ $0,0,\frac{1}{4}$ | (40) $\bar{4}^+ \frac{1}{4},-\frac{1}{4},z;$ $\frac{1}{4},-\frac{1}{4},0$ |
| (41) $\bar{4}^- x,0,\frac{1}{2};$ $\frac{1}{4},0,\frac{1}{2}$ | (42) $a x,y,\bar{y}$ | (43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$ | (44) $\bar{4}^+ x,\frac{1}{4},\frac{1}{4};$ $0,\frac{1}{4},\frac{1}{4}$ |
| (45) $\bar{4}^+ 0,y,\frac{1}{2};$ $0,\frac{1}{4},\frac{1}{2}$ | (46) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^- \frac{1}{4},y,-\frac{1}{4};$ $\frac{1}{4},0,-\frac{1}{4}$ | (48) $b x,y,x$ |

For ($\frac{1}{2},\frac{1}{2},0$)+ set

- | | | | |
|--|--|---|--|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ | (3) 2 0,y,0 | (4) 2 $x,\frac{1}{4},\frac{1}{4}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$ | (6) $3^+ \bar{x},x+\frac{1}{2},\bar{x}$ | (7) $3^+ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+ \bar{x},\bar{x},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$ | (10) $3^- x,\bar{x},\bar{x}$ | (11) $3^- \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ | (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$ | (14) $2 x,\bar{x}+\frac{3}{4},\frac{1}{8}$ | (15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},-\frac{1}{4},z$ | (16) $4^+(0,0,\frac{1}{4})$ $0,\frac{1}{4},z$ |
| (17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$ | (18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,y$ | (19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$ | (20) $4^+(\frac{3}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$ |
| (21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$ | (22) $2(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},x$ | (23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ | (24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$ |
| (25) $\bar{1} \frac{1}{8},\frac{1}{8},\frac{3}{8}$ | (26) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{1}{8}$ | (27) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$ | (28) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y,z$ |
| (29) $\bar{3}^+ x-\frac{1}{2},x,x;$ $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$ | (30) $\bar{3}^+ \bar{x}-\frac{1}{2},x+1,\bar{x};$ $\frac{1}{8},\frac{3}{8},\frac{5}{8}$ | (31) $\bar{3}^+ x-\frac{1}{2},\bar{x}+1,\bar{x};$ $-\frac{1}{8},\frac{5}{8},-\frac{3}{8}$ | (32) $\bar{3}^+ \bar{x}+\frac{3}{2},\bar{x},x;$ $\frac{9}{8},-\frac{3}{8},\frac{3}{8}$ |
| (33) $\bar{3}^- x,x-\frac{1}{2},x;$ $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$ | (34) $\bar{3}^- x+\frac{3}{2},\bar{x}-\frac{3}{2},\bar{x};$ $\frac{3}{8},-\frac{3}{8},\frac{9}{8}$ | (35) $\bar{3}^- \bar{x}+\frac{1}{2},\bar{x}+1,x;$ $\frac{1}{8},\frac{5}{8},\frac{3}{8}$ | (36) $\bar{3}^- \bar{x}+1,x,\bar{x};$ $\frac{5}{8},\frac{3}{8},-\frac{3}{8}$ |
| (37) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$ | (38) $c x,x,z$ | (39) $\bar{4}^- -\frac{1}{4},\frac{1}{4},z;$ $-\frac{1}{4},\frac{1}{4},0$ | (40) $\bar{4}^+ \frac{1}{2},0,z;$ $\frac{1}{2},0,\frac{1}{4}$ |
| (41) $\bar{4}^- x,0,0;$ $\frac{1}{4},0,0$ | (42) $a x,y+\frac{1}{2},\bar{y}$ | (43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$ | (44) $\bar{4}^+ x,\frac{1}{4},-\frac{1}{4};$ $0,\frac{1}{4},-\frac{1}{4}$ |
| (45) $\bar{4}^+ \frac{1}{4},y,\frac{1}{4};$ $\frac{1}{4},0,\frac{1}{4}$ | (46) $b \bar{x},y,x$ | (47) $\bar{4}^- \frac{1}{2},y,0;$ $\frac{1}{2},\frac{1}{4},0$ | (48) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$ |

$Fd\bar{3}c$

O_h^8

$m\bar{3}m$

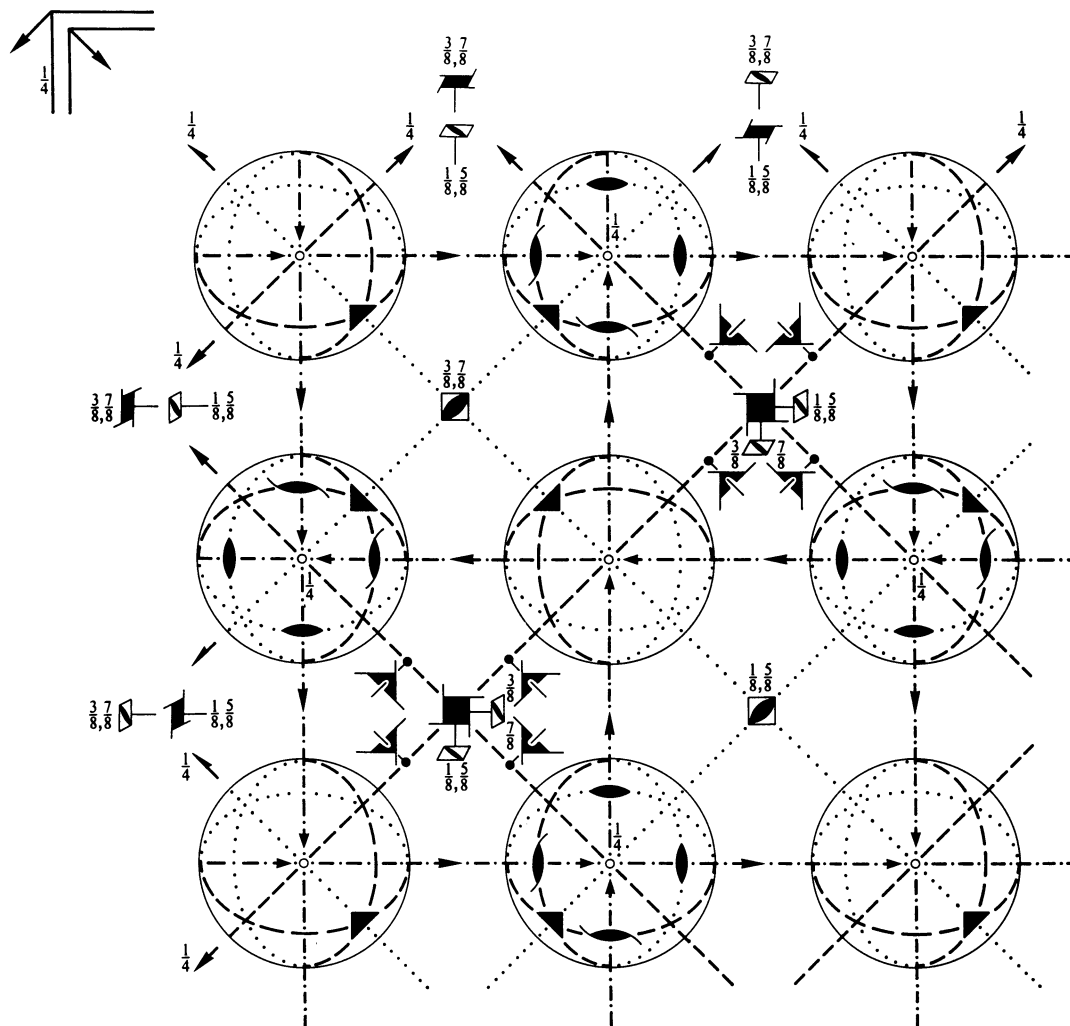
Cubic

No. 228

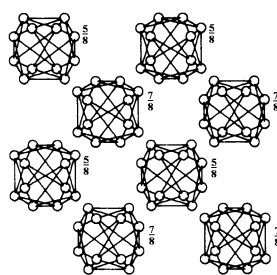
$F4_1/d\bar{3}2/c$

Patterson symmetry $Fm\bar{3}m$

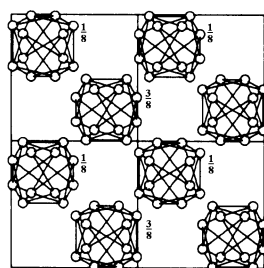
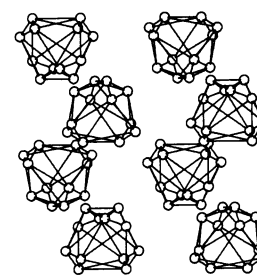
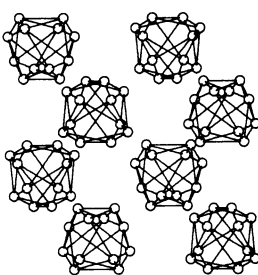
ORIGIN CHOICE 2



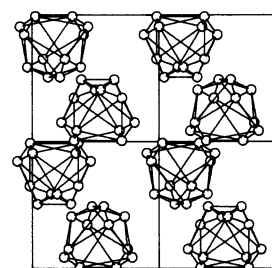
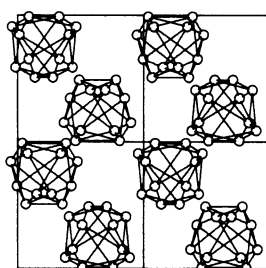
Upper left quadrant only



Upper half of unit cell



Lower half of unit cell



Origin at centre ($\bar{3}$), at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 23

Asymmetric unit $-\frac{1}{8} \leq x \leq \frac{3}{8}; -\frac{1}{8} \leq y \leq 0; -\frac{1}{4} \leq z \leq 0; y \leq \min(\frac{1}{4} - x, x); -y - \frac{1}{4} \leq z \leq y$
Vertices $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{3}{8}, -\frac{1}{8}, -\frac{1}{8}; \frac{1}{4}, 0, 0; 0, 0, 0; \frac{1}{4}, 0, -\frac{1}{4}; 0, 0, -\frac{1}{4}$

Symmetry operations
 (given on page 711)

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions				
	(0, 0, 0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+	($\frac{1}{2}$, 0, $\frac{1}{2}$)+	($\frac{1}{2}$, $\frac{1}{2}$, 0)+	h, k, l permutable General:				
192 <i>h</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z}$ (17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y}$ (21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}, z$ (41) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}, y$ (45) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}, x$	(2) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{3}{4}$ (10) $\bar{y} + \frac{3}{4}, z + \frac{1}{2}, \bar{x} + \frac{1}{4}$ (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (18) $\bar{x}, z + \frac{3}{4}, y + \frac{1}{4}$ (22) $z + \frac{1}{4}, \bar{y}, x + \frac{3}{4}$ (26) $x + \frac{3}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{2}$ (30) $\bar{z} + \frac{1}{2}, x + \frac{3}{4}, y + \frac{1}{4}$ (34) $y + \frac{1}{4}, \bar{z} + \frac{1}{2}, x + \frac{3}{4}$ (38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (42) $x, \bar{z} + \frac{1}{4}, \bar{y} + \frac{3}{4}$ (46) $\bar{z} + \frac{3}{4}, y, \bar{x} + \frac{1}{4}$	(3) $\bar{x} + \frac{3}{4}, y + \frac{1}{2}, \bar{z} + \frac{1}{4}$ (7) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{3}{4}$ (15) $y + \frac{1}{4}, \bar{x}, z + \frac{3}{4}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (23) $\bar{z}, y + \frac{3}{4}, x + \frac{1}{4}$ (27) $x + \frac{1}{4}, \bar{y} + \frac{1}{2}, z + \frac{3}{4}$ (31) $z + \frac{3}{4}, x + \frac{1}{4}, \bar{y} + \frac{1}{2}$ (35) $\bar{y} + \frac{1}{2}, z + \frac{3}{4}, x + \frac{1}{4}$ (39) $\bar{y} + \frac{3}{4}, x, \bar{z} + \frac{1}{4}$ (43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (47) $z, \bar{y} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (8) $\bar{z} + \frac{3}{4}, x + \frac{1}{2}, \bar{y} + \frac{1}{4}$ (12) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{3}{4}, x + \frac{1}{2}$ (16) $\bar{y}, x + \frac{3}{4}, z + \frac{1}{4}$ (20) $x + \frac{1}{4}, \bar{z}, y + \frac{3}{4}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (28) $\bar{x} + \frac{1}{2}, y + \frac{3}{4}, z + \frac{1}{4}$ (32) $z + \frac{1}{4}, \bar{x} + \frac{1}{2}, y + \frac{3}{4}$ (36) $y + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{2}$ (40) $y, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (44) $\bar{x} + \frac{3}{4}, z, \bar{y} + \frac{1}{4}$ (48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k = 2n$ and $h + l, k + l = 2n$ $OkI : k + l = 4n$ and $k, l = 2n$ $hhl : h, l = 2n$ $h00 : h = 4n$				
96 <i>g</i> ..2	$\frac{1}{4}, y, \bar{y}$ $\bar{y}, \frac{1}{4}, y$ $y, \bar{y}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, y$ $y, \frac{3}{4}, \bar{y}$ $\bar{y}, y, \frac{3}{4}$	$0, \bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, 0, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, 0$ $0, y + \frac{1}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, 0, y + \frac{1}{4}$ $y + \frac{1}{4}, y + \frac{1}{2}, 0$	$\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{4}$ $y + \frac{1}{4}, \frac{1}{2}, y + \frac{1}{2}$ $y + \frac{1}{2}, y + \frac{1}{4}, \frac{1}{2}$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \bar{y} + \frac{1}{4}, y + \frac{3}{4}$ $y + \frac{3}{4}, \frac{3}{4}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, y + \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{3}{4}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{1}{4}, y + \frac{3}{4}$ $y + \frac{3}{4}, \bar{y} + \frac{1}{4}, \frac{1}{4}$	no extra conditions				
96 <i>f</i> 2..	$x, \frac{1}{8}, \frac{1}{8}$ $\frac{7}{8}, x + \frac{1}{4}, \frac{7}{8}$ $\bar{x}, \frac{7}{8}, \frac{7}{8}$ $\frac{1}{8}, \bar{x} + \frac{3}{4}, \frac{1}{8}$	$\bar{x} + \frac{1}{4}, \frac{5}{8}, \frac{5}{8}$ $\frac{3}{8}, \bar{x} + \frac{1}{2}, \frac{3}{8}$ $x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}$ $\frac{5}{8}, x + \frac{1}{2}, \frac{5}{8}$	$\frac{1}{8}, x, \frac{1}{8}$ $x + \frac{3}{4}, \frac{3}{8}, \frac{7}{8}$ $\frac{7}{8}, \bar{x}, \frac{7}{8}$ $\bar{x} + \frac{1}{4}, \frac{5}{8}, \frac{1}{8}$	$\frac{5}{8}, \bar{x} + \frac{1}{4}, \frac{5}{8}$ $\bar{x}, \frac{7}{8}, \frac{3}{8}$ $\frac{3}{8}, x + \frac{3}{4}, \frac{3}{8}$ $x, \frac{1}{8}, \frac{5}{8}$	$\frac{1}{8}, \frac{1}{8}, x$ $\frac{7}{8}, \frac{3}{8}, \bar{x}$ $\frac{7}{8}, \frac{7}{8}, \bar{x}$ $\frac{1}{8}, \frac{5}{8}, x$	$\frac{5}{8}, \frac{5}{8}, \bar{x} + \frac{1}{4}$ $\frac{3}{8}, \frac{7}{8}, x + \frac{3}{4}$ $\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}$ $\frac{5}{8}, \frac{1}{8}, \bar{x} + \frac{1}{4}$	$hkl : h + k + l = 4n$		
64 <i>e</i> .3.	x, x, x $x + \frac{3}{4}, x + \frac{1}{4}, \bar{x}$ $\bar{x}, \bar{x}, \bar{x}$ $\bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x$	$\bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{3}{4}, x + \frac{1}{2}, \bar{x} + \frac{1}{4}$ $x + \frac{1}{4}, \bar{x}, x + \frac{3}{4}$ $x + \frac{1}{4}, \bar{x} + \frac{1}{2}, x + \frac{3}{4}$ $\bar{x} + \frac{3}{4}, x, \bar{x} + \frac{1}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}$ $\bar{x}, x + \frac{3}{4}, x + \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x + \frac{3}{4}, x + \frac{1}{4}$ $x, \bar{x} + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$hkl : h = 2n$				
48 <i>d</i> $\bar{4}$..	$\frac{7}{8}, \frac{1}{8}, \frac{1}{8}$ $\frac{7}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{5}{8}$ $\frac{3}{8}, \frac{5}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{1}{8}$ $\frac{5}{8}, \frac{3}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{5}{8}$ $\frac{1}{8}, \frac{7}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{1}{8}, \frac{7}{8}$ $\frac{7}{8}, \frac{3}{8}, \frac{1}{8}$	$\frac{5}{8}, \frac{5}{8}, \frac{3}{8}$ $\frac{3}{8}, \frac{7}{8}, \frac{5}{8}$	$hkl : h + k + l = 4n$		
32 <i>c</i> . $\bar{3}$.	0, 0, 0	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, 0, \frac{3}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$hkl : h, k, l = 4n + 2$ or $h, k, l = 4n$
32 <i>b</i> .32	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, $\frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	0, $\frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{4}, 0$	$\frac{1}{4}, 0, \frac{1}{2}$	$hkl : h, k, l = 4n + 2$ or $h, k, l = 4n$
16 <i>a</i> 23.	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{7}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{5}{8}, \frac{1}{8}$					$hkl : h + k + l = 4n$

ORIGIN CHOICE 2

Symmetry of special projections

Along $[001] p4mm$

$$\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$$

Origin at $\frac{1}{8}, \frac{3}{8}, z$

Along $[111] p6mm$

$$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[110] p2mm$

$$\mathbf{a}' = \frac{1}{4}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	{ [3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	{ [3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	{ [3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	{ [4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (228)

Minimal non-isomorphic supergroups

I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|---|--|--|--|
| (1) 1 | (2) $2(0,0,\frac{1}{2}) \frac{1}{8},\frac{3}{8},z$ | (3) $2(0,\frac{1}{2},0) \frac{3}{8},y,\frac{1}{8}$ | (4) $2(\frac{1}{2},0,0) x,\frac{1}{8},\frac{3}{8}$ |
| (5) $3^+ x,x,x$ | (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3}) \bar{x}+\frac{1}{6},x+\frac{5}{12},\bar{x}$ | (7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3}) x+\frac{7}{12},\bar{x}-\frac{1}{6},\bar{x}$ | (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3}) \bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$ |
| (9) $3^- x,x,x$ | (10) $3^- x+\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$ | (11) $3^- \bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x$ | (12) $3^- \bar{x}-\frac{1}{2},x+\frac{3}{4},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0) x,x-\frac{1}{4},0$ | (14) $2 x,\bar{x}+\frac{1}{2},\frac{1}{4}$ | (15) $4^-(0,0,\frac{3}{4}) \frac{1}{8},-\frac{1}{8},z$ | (16) $4^+(0,0,\frac{1}{4}) -\frac{3}{8},\frac{3}{8},z$ |
| (17) $4^-(\frac{3}{4},0,0) x,\frac{1}{8},-\frac{1}{8}$ | (18) $2(0,\frac{1}{2},\frac{1}{2}) 0,y+\frac{1}{4},y$ | (19) $2 \frac{1}{4},y+\frac{1}{2},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0) x,-\frac{3}{8},\frac{3}{8}$ |
| (21) $4^+(0,\frac{1}{4},0) \frac{3}{8},y,-\frac{3}{8}$ | (22) $2(\frac{1}{2},0,\frac{1}{2}) x-\frac{1}{4},0,x$ | (23) $4^-(0,\frac{3}{4},0) -\frac{1}{8},y,\frac{1}{8}$ | (24) $2 \bar{x}+\frac{1}{2},\frac{1}{4},x$ |
| (25) $\bar{1} 0,0,0$ | (26) $d(\frac{3}{4},\frac{1}{4},0) x,y,\frac{1}{4}$ | (27) $d(\frac{1}{4},0,\frac{3}{4}) x,\frac{1}{4},z$ | (28) $d(0,\frac{3}{4},\frac{1}{4}) \frac{1}{4},y,z$ |
| (29) $\bar{3}^+ x,x,x; 0,0,0$ | (30) $\bar{3}^+ \bar{x}-1,x+\frac{5}{4},\bar{x}; -\frac{1}{4},\frac{1}{2},\frac{3}{4}$ | (31) $\bar{3}^+ x+\frac{1}{4},\bar{x}+1,\bar{x}; \frac{1}{2},\frac{3}{4},-\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x}+\frac{5}{4},\bar{x}+\frac{1}{4},x; \frac{3}{4},-\frac{1}{4},\frac{1}{2}$ |
| (33) $\bar{3}^- x,x,x; 0,0,0$ | (34) $\bar{3}^- x+\frac{3}{4},\bar{x}-1,\bar{x}; 0,-\frac{1}{4},\frac{3}{4}$ | (35) $\bar{3}^- \bar{x}-\frac{1}{4},\bar{x}+\frac{3}{4},x; -\frac{1}{4},\frac{3}{4},0$ | (36) $\bar{3}^- \bar{x}+1,x-\frac{1}{4},\bar{x}; \frac{3}{4},0,-\frac{1}{4}$ |
| (37) $g(-\frac{1}{4},\frac{1}{4},0) x+\frac{1}{2},\bar{x},z$ | (38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) x,x,z$ | (39) $\bar{4}^- \frac{3}{8},\frac{3}{8},z; \frac{3}{8},\frac{3}{8},\frac{1}{8}$ | (40) $\bar{4}^+ \frac{1}{8},\frac{1}{8},z; \frac{1}{8},\frac{1}{8},\frac{3}{8}$ |
| (41) $\bar{4}^- x,\frac{3}{8},\frac{3}{8}; \frac{1}{8},\frac{3}{8},\frac{3}{8}$ | (42) $g(0,-\frac{1}{4},\frac{1}{4}) x,y+\frac{1}{2},\bar{y}$ | (43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) x,y,y$ | (44) $\bar{4}^+ x,\frac{1}{8},\frac{1}{8}; \frac{3}{8},\frac{3}{8},\frac{1}{8}$ |
| (45) $\bar{4}^+ \frac{1}{8},y,\frac{3}{8}; \frac{1}{8},\frac{3}{8},\frac{1}{8}$ | (46) $g(\frac{1}{4},0,-\frac{1}{4}) \bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^- \frac{3}{8},y,\frac{3}{8}; \frac{1}{8},\frac{1}{8},\frac{3}{8}$ | (48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) x,y,x$ |

For (0, $\frac{1}{2},\frac{1}{2}$)+ set

- | | | | |
|---|--|--|--|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) $2 \frac{1}{8},\frac{1}{8},z$ | (3) $2 \frac{3}{8},y,\frac{3}{8}$ | (4) $2(\frac{1}{2},0,0) x,\frac{3}{8},\frac{1}{8}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3}) x-\frac{1}{3},x-\frac{1}{6},x$ | (6) $3^+ \bar{x}+\frac{1}{2},x+\frac{1}{4},\bar{x}$ | (7) $3^+ x+\frac{1}{4},\bar{x},\bar{x}$ | (8) $3^+ \bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3}) x-\frac{1}{6},x+\frac{1}{6},x$ | (10) $3^- x+\frac{3}{4},\bar{x},\bar{x}$ | (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3}) \bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$ | (12) $3^- \bar{x},x+\frac{1}{4},\bar{x}$ |
| (13) $2(\frac{3}{4},\frac{3}{4},0) x,x,\frac{1}{4}$ | (14) $2(\frac{1}{4},-\frac{1}{4},0) x,\bar{x}+\frac{1}{4},0$ | (15) $4^-(0,0,\frac{1}{4}) \frac{3}{8},\frac{1}{8},z$ | (16) $4^+(0,0,\frac{3}{4}) -\frac{1}{8},\frac{1}{8},z$ |
| (17) $4^-(\frac{3}{4},0,0) x,\frac{3}{8},-\frac{1}{8}$ | (18) $2(0,\frac{1}{2},\frac{1}{2}) 0,y-\frac{1}{4},y$ | (19) $2 \frac{1}{4},y,\bar{y}$ | (20) $4^+(\frac{1}{4},0,0) x,\frac{1}{8},\frac{3}{8}$ |
| (21) $4^+(0,\frac{3}{4},0) \frac{5}{8},y,-\frac{1}{8}$ | (22) $2(\frac{1}{4},0,\frac{1}{4}) x,\frac{1}{4},x$ | (23) $4^-(0,\frac{1}{4},0) -\frac{3}{8},y,\frac{3}{8}$ | (24) $2(\frac{1}{4},0,-\frac{1}{4}) \bar{x}+\frac{1}{4},0,x$ |
| (25) $\bar{1} 0,\frac{1}{4},\frac{1}{4}$ | (26) $d(\frac{3}{4},\frac{3}{4},0) x,y,0$ | (27) $d(\frac{1}{4},0,\frac{1}{4}) x,0,z$ | (28) $d(0,\frac{1}{4},\frac{3}{4}) \frac{1}{4},y,z$ |
| (29) $\bar{3}^+ x,x+\frac{1}{2},x; 0,\frac{1}{2},0$ | (30) $\bar{3}^+ \bar{x}-1,x+\frac{3}{4},\bar{x}; -\frac{1}{4},0,\frac{3}{4}$ | (31) $\bar{3}^+ x-\frac{3}{4},\bar{x}+\frac{3}{2},\bar{x}; 0,\frac{3}{4},-\frac{3}{4}$ | (32) $\bar{3}^+ \bar{x}+\frac{1}{4},\bar{x}-\frac{1}{4},x; \frac{1}{4},-\frac{1}{4},0$ |
| (33) $\bar{3}^- x-\frac{1}{2},x-\frac{1}{2},x; 0,0,\frac{1}{2}$ | (34) $\bar{3}^- x+\frac{1}{4},\bar{x}-\frac{1}{2},\bar{x}; 0,-\frac{1}{4},\frac{1}{4}$ | (35) $\bar{3}^- \bar{x}+\frac{1}{4},\bar{x}+\frac{5}{4},x; -\frac{1}{4},\frac{3}{4},\frac{1}{2}$ | (36) $\bar{3}^- \bar{x}+\frac{3}{2},x-\frac{3}{4},\bar{x}; \frac{3}{4},0,-\frac{3}{4}$ |
| (37) $c x+\frac{1}{4},\bar{x},z$ | (38) $g(\frac{1}{4},\frac{1}{4},0) x+\frac{1}{4},x,z$ | (39) $\bar{4}^- \frac{1}{8},\frac{3}{8},z; \frac{1}{8},\frac{3}{8},\frac{3}{8}$ | (40) $\bar{4}^+ \frac{3}{8},\frac{3}{8},z; \frac{1}{8},\frac{3}{8},\frac{1}{8}$ |
| (41) $\bar{4}^- x,-\frac{1}{8},\frac{3}{8}; \frac{1}{8},-\frac{1}{8},\frac{3}{8}$ | (42) $g(0,\frac{1}{4},-\frac{1}{4}) x,y+\frac{1}{2},\bar{y}$ | (43) $a x,y,y$ | (44) $\bar{4}^+ x,\frac{3}{8},\frac{1}{8}; \frac{3}{8},\frac{3}{8},\frac{1}{8}$ |
| (45) $\bar{4}^+ -\frac{1}{8},y,\frac{3}{8}; -\frac{1}{8},\frac{3}{8},\frac{1}{8}$ | (46) $b \bar{x}+\frac{3}{4},y,x$ | (47) $\bar{4}^- \frac{1}{8},y,\frac{1}{8}; \frac{3}{8},\frac{3}{8},\frac{1}{8}$ | (48) $g(\frac{1}{4},0,\frac{1}{4}) x+\frac{1}{4},y,x$ |

For ($\frac{1}{2},0,\frac{1}{2}$)+ set

- | | | | |
|---|---|--|--|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) $2 \frac{3}{8},\frac{3}{8},z$ | (3) $2(0,\frac{1}{2},0) \frac{1}{8},y,\frac{3}{8}$ | (4) $2 x,\frac{1}{8},\frac{1}{8}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3}) x+\frac{1}{6},x-\frac{1}{6},x$ | (6) $3^+ \bar{x},x+\frac{1}{4},\bar{x}$ | (7) $3^+ x+\frac{3}{4},\bar{x},\bar{x}$ | (8) $3^+ \bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3}) x-\frac{1}{6},x-\frac{1}{3},x$ | (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3}) x+\frac{5}{12},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^- \bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$ | (12) $3^- \bar{x},x+\frac{3}{4},\bar{x}$ |
| (13) $2(\frac{1}{4},\frac{1}{4},0) x,x,\frac{1}{4}$ | (14) $2(-\frac{1}{4},\frac{1}{4},0) x,\bar{x}+\frac{1}{4},0$ | (15) $4^-(0,0,\frac{1}{4}) \frac{3}{8},-\frac{3}{8},z$ | (16) $4^+(0,0,\frac{3}{4}) -\frac{1}{8},\frac{5}{8},z$ |
| (17) $4^-(\frac{1}{4},0,0) x,\frac{3}{8},\frac{1}{8}$ | (18) $2(0,\frac{3}{4},\frac{3}{4}) \frac{1}{4},y,y$ | (19) $2(0,\frac{1}{4},-\frac{1}{4}) 0,y+\frac{1}{4},\bar{y}$ | (20) $4^+(\frac{3}{4},0,0) x,-\frac{1}{8},\frac{1}{8}$ |
| (21) $4^+(0,\frac{1}{4},0) \frac{3}{8},y,\frac{1}{8}$ | (22) $2(\frac{1}{2},0,\frac{1}{2}) x+\frac{1}{4},0,x$ | (23) $4^-(0,\frac{3}{4},0) -\frac{1}{8},y,\frac{5}{8}$ | (24) $2 \bar{x},\frac{1}{4},x$ |
| (25) $\bar{1} \frac{1}{4},0,\frac{1}{4}$ | (26) $d(\frac{1}{4},\frac{1}{4},0) x,y,0$ | (27) $d(\frac{3}{4},0,\frac{1}{4}) x,\frac{1}{4},z$ | (28) $d(0,\frac{3}{4},\frac{3}{4}) 0,y,z$ |
| (29) $\bar{3}^+ x-\frac{1}{2},x-\frac{1}{2},x; 0,0,\frac{1}{2}$ | (30) $\bar{3}^+ \bar{x}-\frac{3}{2},x+\frac{3}{4},\bar{x}; -\frac{3}{4},0,\frac{3}{4}$ | (31) $\bar{3}^+ x-\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}; 0,\frac{1}{4},-\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x}+\frac{3}{4},\bar{x}-\frac{1}{4},x; \frac{3}{4},-\frac{1}{4},0$ |
| (33) $\bar{3}^- x+\frac{1}{2},x,x; \frac{1}{2},0,0$ | (34) $\bar{3}^- x+\frac{3}{4},\bar{x}-1,\bar{x}; \frac{1}{2},-\frac{1}{4},\frac{3}{4}$ | (35) $\bar{3}^- \bar{x}-\frac{3}{2},\bar{x}+\frac{3}{2},x; -\frac{3}{4},\frac{3}{4},0$ | (36) $\bar{3}^- \bar{x}+\frac{1}{2},x-\frac{1}{4},\bar{x}; \frac{1}{4},0,-\frac{1}{4}$ |
| (37) $c x+\frac{1}{4},\bar{x},z$ | (38) $g(\frac{1}{4},\frac{1}{4},0) x-\frac{1}{4},x,z$ | (39) $\bar{4}^- \frac{1}{8},\frac{1}{8},z; \frac{1}{8},\frac{1}{8},\frac{3}{8}$ | (40) $\bar{4}^+ \frac{3}{8},-\frac{1}{8},z; \frac{3}{8},-\frac{1}{8},\frac{1}{8}$ |
| (41) $\bar{4}^- x,\frac{1}{8},\frac{5}{8}; \frac{3}{8},\frac{1}{8},\frac{5}{8}$ | (42) $a x,y+\frac{1}{4},\bar{y}$ | (43) $g(0,\frac{1}{4},\frac{1}{4}) x,y+\frac{1}{4},y$ | (44) $\bar{4}^+ x,\frac{3}{8},\frac{3}{8}; \frac{1}{8},\frac{3}{8},\frac{3}{8}$ |
| (45) $\bar{4}^+ \frac{1}{8},y,\frac{5}{8}; \frac{3}{8},\frac{3}{8},\frac{5}{8}$ | (46) $g(-\frac{1}{4},0,\frac{1}{4}) \bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^- \frac{3}{8},y,-\frac{1}{8}; \frac{3}{8},\frac{1}{8},-\frac{1}{8}$ | (48) $b x,y,x$ |

For ($\frac{1}{2},\frac{1}{2},0$)+ set

- | | | | |
|---|--|--|---|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2}) \frac{3}{8},\frac{3}{8},z$ | (3) $2 \frac{1}{8},y,\frac{1}{8}$ | (4) $2 x,\frac{3}{8},\frac{3}{8}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3}) x+\frac{1}{6},x+\frac{1}{3},x$ | (6) $3^+ \bar{x},x+\frac{3}{4},\bar{x}$ | (7) $3^+ x+\frac{3}{4},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+ \bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3}) x+\frac{1}{3},x+\frac{1}{6},x$ | (10) $3^- x+\frac{1}{4},\bar{x},\bar{x}$ | (11) $3^- \bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$ | (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3}) \bar{x}-\frac{1}{6},x+\frac{7}{12},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},0$ | (14) $2 x,\bar{x},\frac{1}{4}$ | (15) $4^-(0,0,\frac{3}{4}) \frac{5}{8},-\frac{1}{8},z$ | (16) $4^+(0,0,\frac{1}{4}) \frac{1}{8},\frac{3}{8},z$ |
| (17) $4^-(\frac{1}{4},0,0) x,\frac{3}{8},-\frac{3}{8}$ | (18) $2(0,\frac{1}{4},\frac{1}{4}) \frac{1}{4},y,y$ | (19) $2(0,-\frac{1}{4},\frac{1}{4}) 0,y+\frac{1}{4},\bar{y}$ | (20) $4^+(\frac{3}{4},0,0) x,-\frac{1}{8},\frac{5}{8}$ |
| (21) $4^+(0,\frac{3}{4},0) \frac{1}{8},y,-\frac{1}{8}$ | (22) $2(\frac{3}{4},0,\frac{3}{4}) x,\frac{1}{4},x$ | (23) $4^-(0,\frac{1}{4},0) \frac{1}{8},y,\frac{3}{8}$ | (24) $2(-\frac{1}{4},0,\frac{1}{4}) \bar{x}+\frac{1}{4},0,x$ |
| (25) $\bar{1} \frac{1}{4},\frac{1}{4},0$ | (26) $d(\frac{1}{4},\frac{3}{4},0) x,y,\frac{1}{4}$ | (27) $d(\frac{3}{4},0,\frac{3}{4}) x,0,z$ | (28) $d(0,\frac{1}{4},\frac{1}{4}) 0,y,z$ |
| (29) $\bar{3}^+ x+\frac{1}{2},x,x; \frac{1}{2},0,0$ | (30) $\bar{3}^+ \bar{x}-\frac{1}{2},x+\frac{1}{4},\bar{x}; -\frac{1}{4},0,\frac{1}{4}$ | (31) $\bar{3}^+ x-\frac{1}{4},\bar{x}+1,\bar{x}; 0,\frac{3}{4},-\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x}+\frac{3}{4},\bar{x}-\frac{3}{4},x; \frac{3}{4},-\frac{3}{4},0$ |
| (33) $\bar{3}^- x,x+\frac{1}{2},x; 0,\frac{1}{2},0$ | (34) $\bar{3}^- x+\frac{3}{4},\bar{x}-\frac{3}{2},\bar{x}; 0,-\frac{3}{4},\frac{3}{4}$ | (35) $\bar{3}^- \bar{x}-\frac{1}{4},\bar{x}+\frac{1}{4},x; -\frac{1}{4},\frac{1}{4},0$ | (36) $\bar{3}^- \bar{x}+1,x+\frac{1}{4},\bar{x}; \frac{3}{4},\frac{1}{2},-\frac{1}{4}$ |
| (37) $g(\frac{1}{4},-\frac{1}{4},0) x+\frac{1}{2},\bar{x},z$ | (38) $c x,x,z$ | (39) $\bar{4}^- \frac{1}{8},\frac{3}{8},z; -\frac{1}{8},\frac{3}{8},\frac{1}{8}$ | (40) $\bar{4}^+ \frac{5}{8},\frac{3}{8},z; \frac{5}{8},\frac{1}{8},\frac{3}{8}$ |
| (41) $\bar{4}^- x,\frac{1}{8},\frac{1}{8}; \frac{3}{8},\frac{1}{8},\frac{1}{8}$ | (42) $a x,y+\frac{3}{4},\bar{y}$ | (43) $g(0,\frac{1}{4},\frac{1}{4}) x,y-\frac{1}{4},y$ | (44) $\bar{4}^+ x,\frac{3}{8},-\frac{1}{8}; \frac{1}{8},\frac{3}{8},-\frac{1}{8}$ |
| (45) $\bar{4}^+ \frac{3}{8},y,\frac{3}{8}; \frac{3}{8},\frac{1}{8},\frac{3}{8}$ | (46) $b \bar{x}+\frac{1}{4},y,x$ | (47) $\bar{4}^- \frac{5}{8},y,\frac{1}{8}; \frac{5}{8},\frac{3}{8},\frac{1}{8}$ | (48) $g(\frac{1}{4},0,\frac{1}{4}) x-\frac{1}{4},y,x$ |

$I m \bar{3} m$

O_h^9

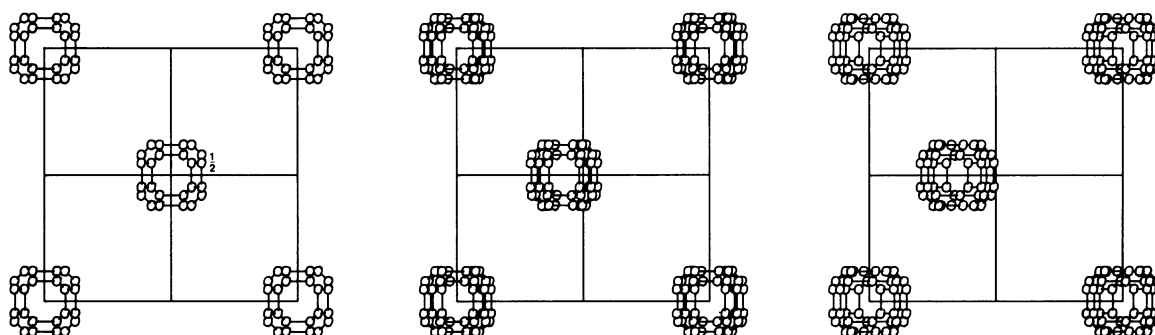
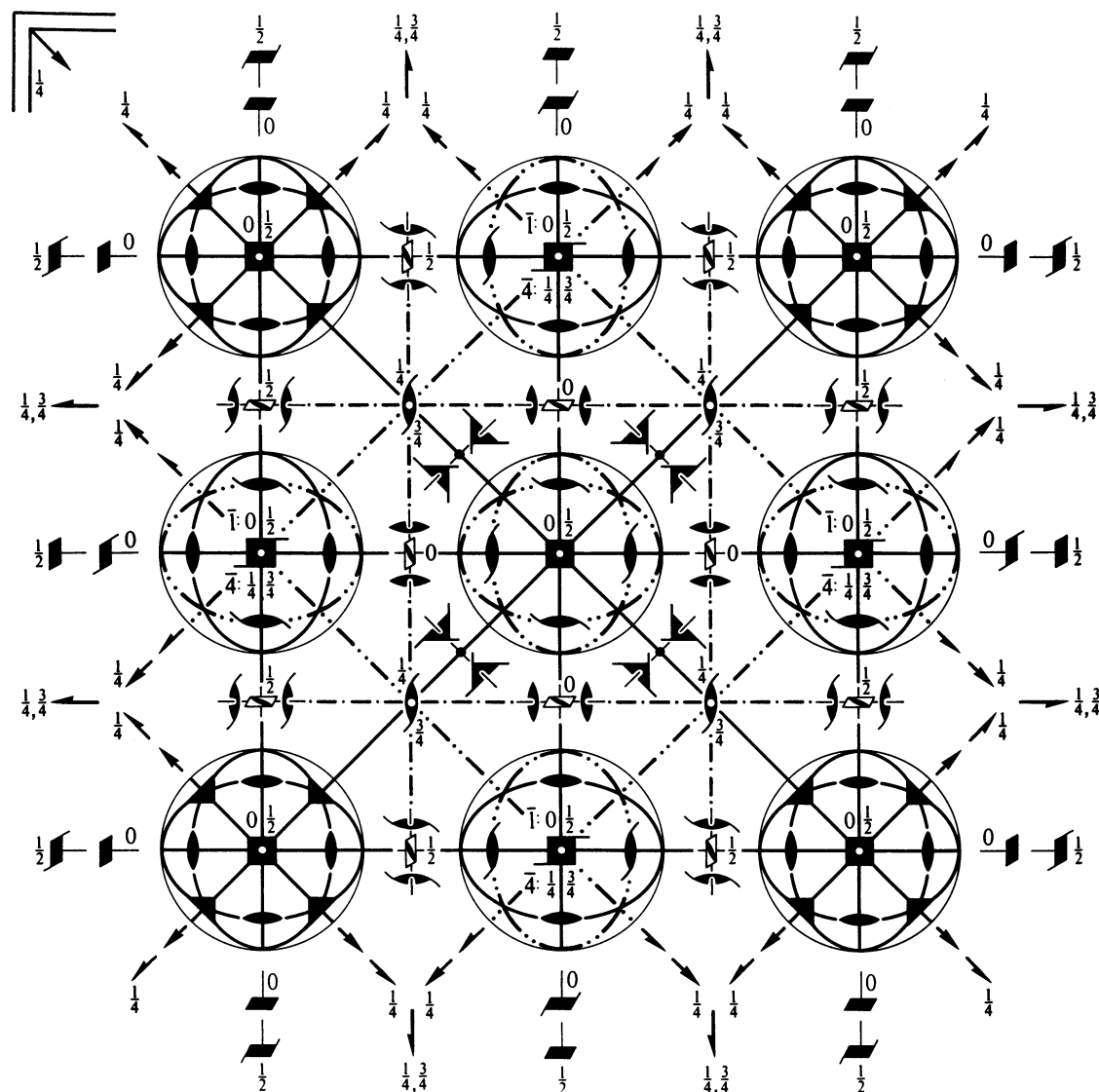
$m \bar{3} m$

Cubic

No. 229

$I 4/m \bar{3} 2/m$

Patterson symmetry $I m \bar{3} m$



Origin at centre ($m \bar{3} m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; y \leq x; z \leq \min(\frac{1}{2} - x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Symmetry operations

(given on page 714)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$						Reflection conditions
96 <i>l</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) y, x, \bar{z} (17) x, z, \bar{y} (21) z, y, \bar{x} (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) \bar{y}, \bar{x}, z (41) \bar{x}, \bar{z}, y (45) \bar{z}, \bar{y}, x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y}, \bar{x}, \bar{z}$ (18) \bar{x}, z, y (22) z, \bar{y}, x (26) x, y, \bar{z} (30) \bar{z}, x, y (34) y, \bar{z}, x (38) y, x, z (42) x, \bar{z}, \bar{y} (46) \bar{z}, y, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, z (19) $\bar{x}, \bar{z}, \bar{y}$ (23) \bar{z}, y, x (27) x, \bar{y}, z (31) \bar{z}, x, y (35) \bar{y}, z, x (39) \bar{y}, x, \bar{z} (43) x, z, y (47) z, \bar{y}, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, z (20) x, \bar{z}, y (24) $\bar{z}, \bar{y}, \bar{x}$ (28) \bar{x}, y, z (32) z, \bar{x}, y (36) y, z, \bar{x} (40) y, \bar{x}, \bar{z} (44) \bar{x}, z, \bar{y} (48) z, y, x			$hkl : h + k + l = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$
48 <i>k</i> . . <i>m</i>	x, x, z \bar{z}, \bar{x}, x x, x, \bar{z} $\bar{x}, \bar{z}, \bar{x}$	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x} $\bar{x}, \bar{x}, \bar{z}$ x, \bar{z}, x	\bar{x}, x, \bar{z} x, z, x x, \bar{x}, z z, x, \bar{x}	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x} \bar{x}, x, z z, \bar{x}, x	z, x, x x, \bar{z}, \bar{x} x, z, \bar{x} \bar{z}, x, x	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x \bar{x}, z, x $\bar{z}, \bar{x}, \bar{x}$	no extra conditions
48 <i>j</i> <i>m</i> . .	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions
48 <i>i</i> . . 2	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$			no extra conditions
24 <i>h</i> <i>m</i> . <i>m</i> 2	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions
24 <i>g</i> <i>m</i> <i>m</i> 2 . .	$x, 0, \frac{1}{2}$ $0, x, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, x, 0$ $x, \frac{1}{2}, 0$	$\frac{1}{2}, \bar{x}, 0$ $\bar{x}, \frac{1}{2}, 0$	$0, \frac{1}{2}, x$ $\frac{1}{2}, 0, \bar{x}$	$0, \frac{1}{2}, \bar{x}$ $\frac{1}{2}, 0, x$	no extra conditions
16 <i>f</i> . 3 <i>m</i>	x, x, x x, x, \bar{x}	\bar{x}, \bar{x}, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x			no extra conditions
12 <i>e</i> 4 <i>m</i> . <i>m</i>	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions
12 <i>d</i> $\bar{4}$ <i>m</i> . 2	$\frac{1}{4}, 0, \frac{1}{2}$	$\frac{3}{4}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{3}{4}, 0$	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	no extra conditions
8 <i>c</i> . $\bar{3}$ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : k, l = 2n$
6 <i>b</i> 4/ <i>m</i> <i>m</i> . <i>m</i>	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
2 <i>a</i> <i>m</i> $\bar{3}$ <i>m</i>	$0, 0, 0$						no extra conditions

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0,0,z

Along [111] $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** [2] $I\bar{4}3m$ (217) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
 [2] $I432$ (211) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
 [2] $Im\bar{3}1$ ($Im\bar{3}$, 204) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
 { [3] $I4/m12/m(I4/mmm, 139)$ (1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
 [3] $I4/m12/m(I4/mmm, 139)$ (1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
 [3] $I4/m12/m(I4/mmm, 139)$ (1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
 { [4] $I1\bar{3}2/m(R\bar{3}m, 166)$ (1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
 [4] $I1\bar{3}2/m(R\bar{3}m, 166)$ (1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
 [4] $I1\bar{3}2/m(R\bar{3}m, 166)$ (1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
 [4] $I1\bar{3}2/m(R\bar{3}m, 166)$ (1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
- IIa** [2] $Pn\bar{3}m$ (224) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $Pm\bar{3}n$ (223) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $Pn\bar{3}n$ (222) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; (25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $Pm\bar{3}m$ (221) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [27] $Im\bar{3}m$ ($a' = 3a, b' = 3b, c' = 3c$) (229)

Minimal non-isomorphic supergroups

- I** none
II [4] $Pm\bar{3}m$ ($a' = \frac{1}{2}a, b' = \frac{1}{2}b, c' = \frac{1}{2}c$) (221)

Symmetry operations

For (0,0,0)+ set

- | | | | |
|----------------------------------|---|---|--|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x},x,\bar{x} | (7) 3 ⁺ x, \bar{x},\bar{x} | (8) 3 ⁺ \bar{x},\bar{x},x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x},\bar{x} | (11) 3 ⁻ \bar{x},\bar{x},x | (12) 3 ⁻ \bar{x},x,\bar{x} |
| (13) 2 x,x,0 | (14) 2 x, \bar{x} ,0 | (15) 4 ⁻ 0,0,z | (16) 4 ⁺ 0,0,z |
| (17) 4 ⁻ x,0,0 | (18) 2 0,y,y | (19) 2 0,y, \bar{y} | (20) 4 ⁺ x,0,0 |
| (21) 4 ⁺ 0,y,0 | (22) 2 x,0,x | (23) 4 ⁻ 0,y,0 | (24) 2 \bar{x} ,0,x |
| (25) $\bar{1}$ 0,0,0 | (26) m x,y,0 | (27) m x,0,z | (28) m 0,y,z |
| (29) $\bar{3}^+$ x,x,x; 0,0,0 | (30) $\bar{3}^+$ \bar{x},x,\bar{x} ; 0,0,0 | (31) $\bar{3}^+$ x, \bar{x},\bar{x} ; 0,0,0 | (32) $\bar{3}^+$ \bar{x},\bar{x},x ; 0,0,0 |
| (33) $\bar{3}^-$ x,x,x; 0,0,0 | (34) $\bar{3}^-$ x, \bar{x},\bar{x} ; 0,0,0 | (35) $\bar{3}^-$ \bar{x},\bar{x},x ; 0,0,0 | (36) $\bar{3}^-$ \bar{x},x,\bar{x} ; 0,0,0 |
| (37) m x, \bar{x} ,z | (38) m x,x,z | (39) 4 ⁻ 0,0,z; 0,0,0 | (40) 4 ⁺ 0,0,z; 0,0,0 |
| (41) 4 ⁻ x,0,0; 0,0,0 | (42) m x,y, \bar{y} | (43) m x,y,y | (44) 4 ⁺ x,0,0; 0,0,0 |
| (45) 4 ⁺ 0,y,0; 0,0,0 | (46) m \bar{x},y,x | (47) 4 ⁻ 0,y,0; 0,0,0 | (48) m x,y,x |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0,\frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (3) $2(0,\frac{1}{2},0) \frac{1}{4}, y, \frac{1}{4}$ | (4) $2(\frac{1}{2},0,0) x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, x$ | (6) $3^+(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}) \bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$ | (7) $3^+(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}) x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$ | (8) $3^+(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}) \bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, x$ | (10) $3^-(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}) x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$ | (11) $3^-(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}) \bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$ | (12) $3^-(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}) \bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, \frac{1}{4}$ | (14) 2 x, $\bar{x} + \frac{1}{2}, \frac{1}{4}$ | (15) $4^-(0,0,\frac{1}{2}) \frac{1}{2}, 0, z$ | (16) $4^+(0,0,\frac{1}{2}) 0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) x, \frac{1}{2}, 0$ | (18) $2(0,\frac{1}{2}, \frac{1}{2}) \frac{1}{4}, y, y$ | (19) $2 \frac{1}{4}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) x, 0, \frac{1}{2}$ |
| (21) $4^+(0,\frac{1}{2}, 0) \frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x, \frac{1}{4}, x$ | (23) $4^-(0,\frac{1}{2}, 0) 0, y, \frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ |
| (25) $\bar{1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (26) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, \frac{1}{4}$ | (27) $n(\frac{1}{2}, 0, \frac{1}{2}) x, \frac{1}{4}, z$ | (28) $n(0, \frac{1}{2}, \frac{1}{2}) \frac{1}{4}, y, z$ |
| (29) $\bar{3}^+ x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (30) $\bar{3}^+ \bar{x} - 1, x + 1, \bar{x}; -\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ | (31) $\bar{3}^+ x, \bar{x} + 1, \bar{x}; \frac{1}{4}, \frac{3}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+ \bar{x} + 1, \bar{x}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{4}$ |
| (33) $\bar{3}^- x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (34) $\bar{3}^- x + 1, \bar{x} - 1, \bar{x}; \frac{1}{4}, -\frac{1}{4}, \frac{3}{4}$ | (35) $\bar{3}^- \bar{x}, \bar{x} + 1, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ | (36) $\bar{3}^- \bar{x} + 1, x, \bar{x}; \frac{3}{4}, \frac{1}{4}, -\frac{1}{4}$ |
| (37) c $x + \frac{1}{2}, \bar{x}, z$ | (38) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, z$ | (39) $4^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ | (40) $4^+ \frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ |
| (41) $4^- x, 0, \frac{1}{2}; \frac{1}{4}, 0, \frac{1}{2}$ | (42) a $x, y + \frac{1}{2}, \bar{y}$ | (43) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, y$ | (44) $4^+ x, \frac{1}{2}, 0; \frac{1}{4}, \frac{1}{2}, 0$ |
| (45) $4^+ 0, y, \frac{1}{2}; 0, \frac{1}{4}, \frac{1}{2}$ | (46) b $\bar{x} + \frac{1}{2}, y, x$ | (47) $4^- \frac{1}{2}, y, 0; \frac{1}{2}, \frac{1}{4}, 0$ | (48) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, x$ |

$Ia\bar{3}d$

O_h^{10}

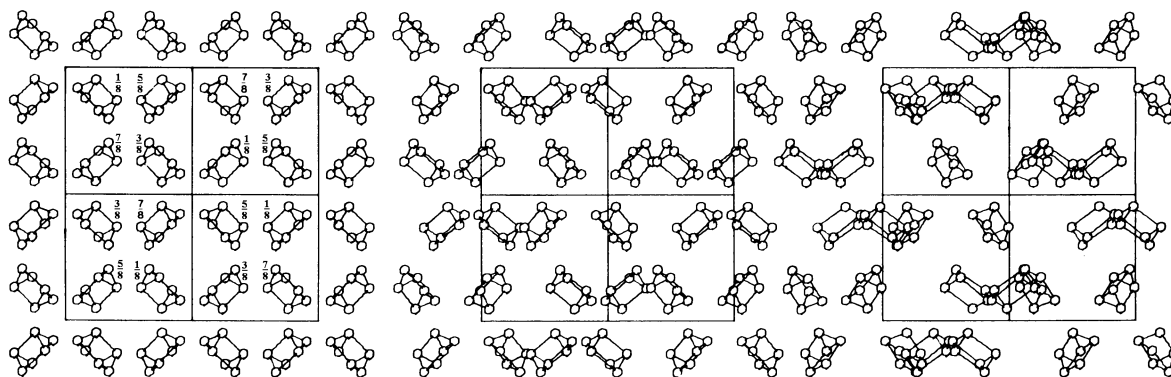
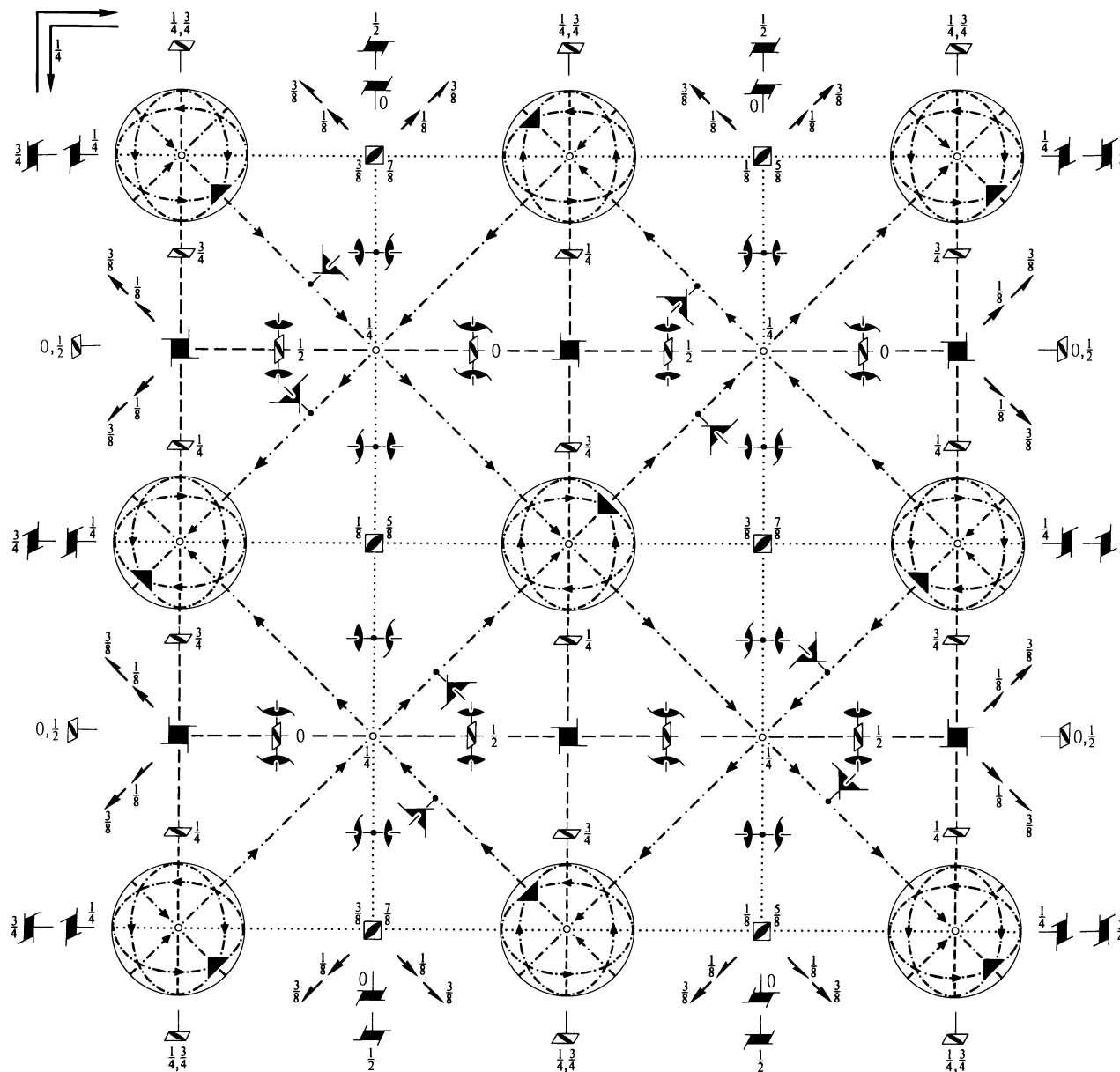
$m\bar{3}m$

Cubic

No. 230

$I 4_1/a \bar{3} 2/d$

Patterson symmetry $Im\bar{3}m$



Origin at centre ($\bar{3}$)

Asymmetric unit

$$-\frac{1}{2} \leq x \leq \frac{1}{2}; \quad -\frac{1}{2} \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad \max(x, -x, y, -y) \leq z$$

Vertices

$$0, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{4} \quad -\frac{1}{2}, \frac{1}{2}, \frac{1}{4} \quad -\frac{1}{2}, -\frac{1}{2}, \frac{1}{4} \quad \frac{1}{2}, -\frac{1}{2}, \frac{1}{4}$$

$$\frac{1}{2}, \frac{1}{2}, \frac{3}{4} \quad -\frac{1}{2}, \frac{1}{2}, \frac{3}{4} \quad -\frac{1}{2}, -\frac{1}{2}, \frac{3}{4} \quad \frac{1}{2}, -\frac{1}{2}, \frac{3}{4}$$

Symmetry operations

(given on page 715)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)**Positions**Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

Reflection conditions

 h,k,l permutable

General:

96	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$hkl : h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$OkL : k,l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	$hhl : 2h+l=4n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	$h00 : h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$	
			(25) \bar{x},\bar{y},\bar{z}	(26) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(27) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	
			(29) \bar{z},\bar{x},\bar{y}	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(31) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(32) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(33) \bar{y},\bar{z},\bar{x}	(34) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(36) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(38) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(39) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(40) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(42) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(44) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$	
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(46) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(47) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$	

Special: as above, plus

48	g	$\dots 2$	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$	$hkl : h=2n+1$
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$	$y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$	or $h=4n$
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$	
			$\frac{7}{8},\bar{y},y+\frac{3}{4}$	$\frac{5}{8},y,y+\frac{1}{4}$	$\frac{1}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$	
			$y+\frac{3}{4},\frac{7}{8},\bar{y}$	$y+\frac{1}{4},\frac{5}{8},y$	$\bar{y}+\frac{3}{4},\frac{1}{8},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{4},\frac{3}{8},y+\frac{1}{2}$	
			$\bar{y},y+\frac{3}{4},\frac{7}{8}$	$y,y+\frac{1}{4},\frac{5}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{1}{8}$	$y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{8}$	

48	f	$2 \dots$	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	$hkl : 2h+l=4n$
			$\frac{3}{4},x+\frac{1}{4},0$	$\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$	$x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\bar{x}+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$	
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x},0$	$\frac{1}{4},x+\frac{1}{2},0$	$0,\frac{3}{4},\bar{x}$	$0,\frac{1}{4},x+\frac{1}{2}$	
			$\frac{1}{4},\bar{x}+\frac{3}{4},0$	$\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$x+\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},x+\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\bar{x}+\frac{1}{4}$	

32	e	$\dots 3 \dots$	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	$hkl : h=2n+1$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	or $h+k+l=4n$
			\bar{x},\bar{x},\bar{x}	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$	
			$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$	$x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$	

24	d	$\bar{4} \dots$	$\frac{3}{8},0,\frac{1}{4}$	$\frac{1}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{3}{8},0$	$\frac{3}{4},\frac{1}{8},0$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{1}{8}$	$hkl : h,k=2n, h+k+l=4n$ or $h,k=2n+1, l=4n+2$ or $h=8n, k=8n+4$ and $h+k+l=4n+2$
			$\frac{3}{4},\frac{5}{8},0$	$\frac{3}{4},\frac{3}{8},\frac{1}{2}$	$\frac{1}{8},\frac{1}{2},\frac{1}{4}$	$\frac{7}{8},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{7}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	
24	c	$2 \dots 22$	$\frac{1}{8},0,\frac{1}{4}$	$\frac{3}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{8},0$	$\frac{3}{4},\frac{3}{8},0$	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$	
			$\frac{7}{8},0,\frac{3}{4}$	$\frac{5}{8},0,\frac{1}{4}$	$\frac{3}{4},\frac{7}{8},0$	$\frac{1}{4},\frac{5}{8},0$	$0,\frac{3}{4},\frac{7}{8}$	$0,\frac{1}{4},\frac{5}{8}$	

16	b	$\dots 3 2$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$	$hkl : h,k=2n+1, l=4n+2$ or $h,k,l=4n$
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16	a	$\dots \bar{3}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$hkl : h,k=2n, h+k+l=4n$
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(Continued on page 715)

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{4}, 0, z$

Along [111] $p6mm$
 $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
 Origin at x, x, x

Along [110] $c2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, x + \frac{1}{4}, \frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}3d$ (220)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $I4_132$ (214)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Ia\bar{3}1$ ($Ia\bar{3}$, 206)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	{ [3] $I4_1/a12/d$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	{ [3] $I4_1/a12/d$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	{ [3] $I4_1/a12/d$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	{ [4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	{ [4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	{ [4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	{ [4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Ia\bar{3}d$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (230)

Minimal non-isomorphic supergroups

I none

II [4] $Pm\bar{3}n$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (223)

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}, 0, z$	(3) $2(0,\frac{1}{2},0)$ $0, y, \frac{1}{4}$	(4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$
(5) $3^+ x, x, x$	(6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$	(7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$	(8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$
(9) $3^- x, x, x$	(10) $3^- (-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$	(11) $3^- (\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$	(12) $3^- (\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$
(13) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x - \frac{1}{4}, \frac{3}{8}$	(14) $2(x, \bar{x} + \frac{3}{4}, \frac{3}{8})$	(15) $4^-(0, 0, \frac{3}{4})$ $\frac{1}{4}, 0, z$	(16) $4^+(0, 0, \frac{1}{4})$ $-\frac{1}{4}, \frac{1}{2}, z$
(17) $4^-(\frac{3}{4}, 0, 0)$ $x, \frac{1}{4}, 0$	(18) $2(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{8}, y + \frac{1}{4}, y$	(19) $2(\frac{3}{8}, y + \frac{3}{4}, \bar{y})$	(20) $4^+(\frac{1}{4}, 0, 0)$ $x, -\frac{1}{4}, \frac{1}{2}$
(21) $4^+(0, \frac{1}{4}, 0)$ $\frac{1}{2}, y, -\frac{1}{4}$	(22) $2(\frac{1}{2}, 0, \frac{1}{2})$ $x - \frac{1}{4}, \frac{1}{8}, x$	(23) $4^-(0, \frac{3}{4}, 0)$ $0, y, \frac{1}{4}$	(24) $2(\bar{x} + \frac{1}{4}, \frac{3}{8}, x)$
(25) $\bar{1}$ $0, 0, 0$	(26) a $x, y, \frac{1}{4}$	(27) c $x, \frac{1}{4}, z$	(28) b $\frac{1}{4}, y, z$
(29) $\bar{3}^+ x, x, x; 0, 0, 0$	(30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + 1, \bar{x}; 0, \frac{1}{2}, \frac{1}{2}$	(31) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \frac{1}{2}, \frac{1}{2}, 0$	(32) $\bar{3}^+ \bar{x} + 1, \bar{x} + \frac{1}{2}, x; \frac{1}{2}, 0, \frac{1}{2}$
(33) $\bar{3}^- x, x, x; 0, 0, 0$	(34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; 0, 0, \frac{1}{2}$	(35) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; 0, \frac{1}{2}, 0$	(36) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{2}, 0, 0$
(37) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{2}, \bar{x}, z$	(38) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ x, x, z	(39) $\bar{4}^- 0, \frac{3}{4}, z; 0, \frac{3}{4}, \frac{1}{8}$	(40) $\bar{4}^+ \frac{1}{2}, -\frac{1}{4}, z; \frac{1}{2}, -\frac{1}{4}, \frac{3}{8}$
(41) $\bar{4}^- x, 0, \frac{3}{4}; \frac{1}{8}, 0, \frac{3}{4}$	(42) $d(\frac{3}{4}, -\frac{1}{4}, \frac{1}{4})$ $x, y + \frac{1}{2}, \bar{y}$	(43) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ x, y, y	(44) $\bar{4}^+ x, \frac{1}{2}, -\frac{1}{4}; \frac{3}{8}, \frac{1}{2}, -\frac{1}{4}$
(45) $\bar{4}^+ -\frac{1}{4}, y, \frac{1}{2}; -\frac{1}{4}, \frac{3}{8}, \frac{1}{2}$	(46) $d(\frac{1}{4}, \frac{3}{4}, -\frac{1}{4})$ $\bar{x} + \frac{1}{2}, y, x$	(47) $\bar{4}^- \frac{3}{4}, y, 0; \frac{3}{4}, \frac{3}{8}, 0$	(48) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ x, y, x

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

(1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(2) 2 $0, \frac{1}{4}, z$	(3) 2 $\frac{1}{4}, y, 0$	(4) 2 $x, 0, \frac{1}{4}$
(5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, x	(6) $3^+(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$	(7) $3^+(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$	(8) $3^+(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$
(9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, x	(10) $3^-(\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6})$ $x + \frac{1}{6}, \bar{x} + \frac{1}{6}, \bar{x}$	(11) $3^-(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{6}, x$	(12) $3^-(\frac{1}{6}, \frac{1}{6}, -\frac{1}{6})$ $\bar{x} - \frac{1}{6}, x + \frac{1}{3}, \bar{x}$
(13) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x + \frac{1}{4}, \frac{3}{8}$	(14) $2(x, \bar{x} + \frac{1}{4}, \frac{3}{8})$	(15) $4^-(0, 0, \frac{1}{4})$ $\frac{3}{4}, 0, z$	(16) $4^+(0, 0, \frac{3}{4})$ $\frac{1}{4}, \frac{1}{2}, z$
(17) $4^-(\frac{1}{4}, 0, 0)$ $x, \frac{3}{4}, 0$	(18) $2(0, \frac{1}{2}, \frac{1}{2})$ $\frac{3}{8}, y - \frac{1}{4}, y$	(19) $2(\frac{1}{8}, y + \frac{1}{4}, \bar{y})$	(20) $4^+(\frac{3}{4}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{2}$
(21) $4^+(0, \frac{3}{4}, 0)$ $\frac{1}{2}, y, \frac{1}{4}$	(22) $2(\frac{1}{2}, 0, \frac{1}{2})$ $x + \frac{1}{4}, \frac{3}{8}, x$	(23) $4^-(0, \frac{1}{4}, 0)$ $0, y, \frac{3}{4}$	(24) $2(\bar{x} + \frac{1}{4}, \frac{1}{8}, x)$
(25) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(26) b $x, y, 0$	(27) a $x, 0, z$	(28) c $0, y, z$
(29) $\bar{3}^+ x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x, \bar{x}; -\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$	(31) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; -\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$	(32) $\bar{3}^+ \bar{x}, \bar{x} - \frac{1}{2}, x; \frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$
(33) $\bar{3}^- x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$	(35) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(36) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$
(37) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{2}, \bar{x}, z$	(38) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ x, x, z	(39) $\bar{4}^- 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$	(40) $\bar{4}^+ \frac{1}{2}, \frac{1}{4}, z; \frac{1}{2}, \frac{1}{4}, \frac{3}{8}$
(41) $\bar{4}^- x, 0, \frac{1}{4}; \frac{3}{8}, 0, \frac{1}{4}$	(42) $d(\frac{1}{4}, \frac{1}{4}, -\frac{1}{4})$ $x, y + \frac{1}{2}, \bar{y}$	(43) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ x, y, y	(44) $\bar{4}^+ x, \frac{1}{2}, \frac{1}{4}; \frac{1}{8}, \frac{1}{2}, \frac{1}{4}$
(45) $\bar{4}^+ \frac{1}{4}, y, \frac{1}{2}; \frac{1}{4}, \frac{1}{8}, \frac{1}{2}$	(46) $d(-\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $\bar{x} + \frac{1}{2}, y, x$	(47) $\bar{4}^- \frac{1}{4}, y, 0; \frac{1}{4}, \frac{3}{8}, 0$	(48) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ x, y, x