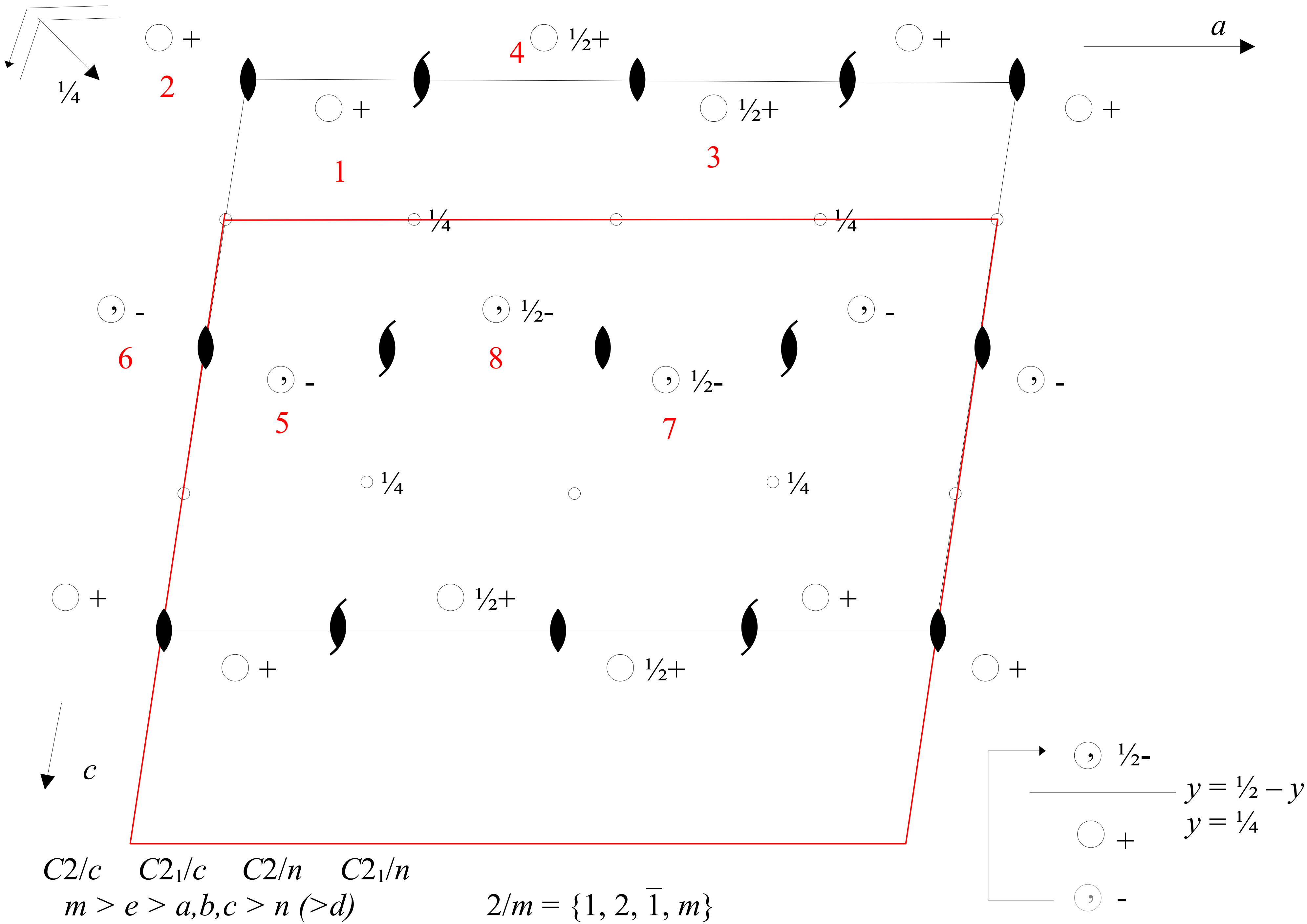
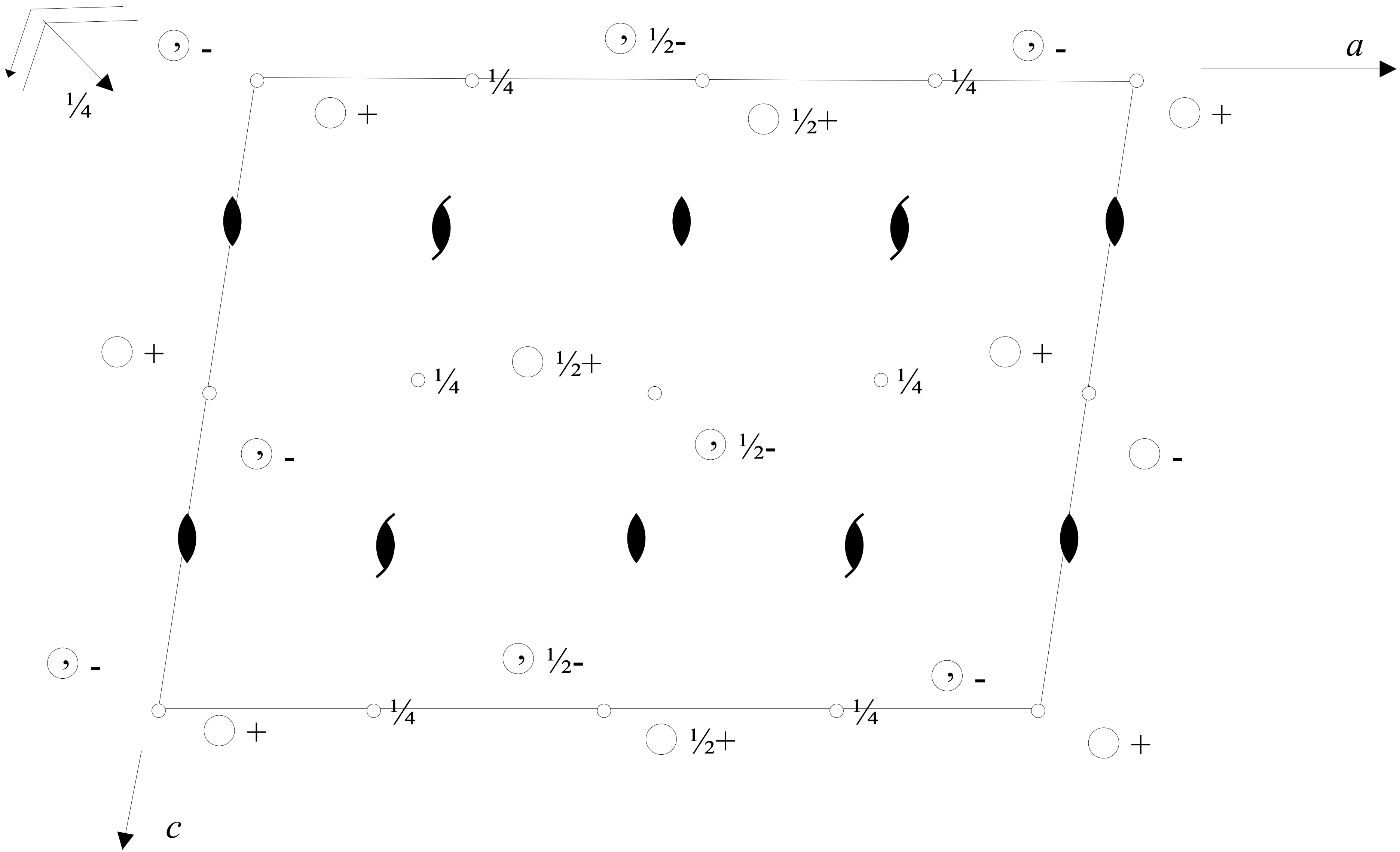


$C2/c$ $C2_1/c$ $C2/n$ $C2_1/n$

$m > e > a,b,c > n\ (>d)$

$2/m = \{1, 2, \bar{1}, m\}$



a
c
¼
½+
½-
+
-

(000)+ (½½0)+

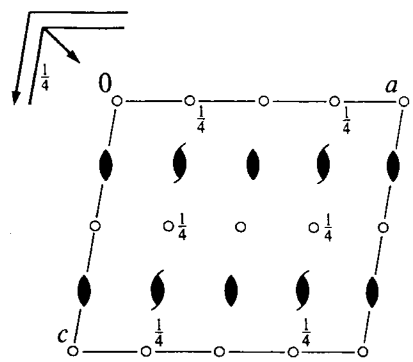
Multiplicity	Site-symmetry group	Coordinates	
8	1	xyz, $x\bar{y}\tfrac{1}{2}+z$, $\bar{x}\bar{y}\bar{z}$, $\bar{x}y\tfrac{1}{2}-z$	
4	2	$0y\tfrac{1}{4}$, $0\bar{y}\tfrac{3}{4}$	
4	$\bar{1}$	000, 00½	
4	$\bar{1}$	0½0, 0½½	
4	$\bar{1}$	¼¼0, ¼¾½, (¾¾0, ¾¼½)	Related by (½½0)+, we do not write these coordinates explicitly
4	$\bar{1}$	¼¾0, ¼¼½	

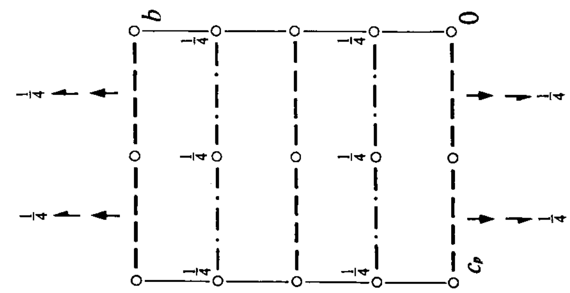
International Tables for Crystallography (2006). Vol. A, Space group 15, pp. 192–199.

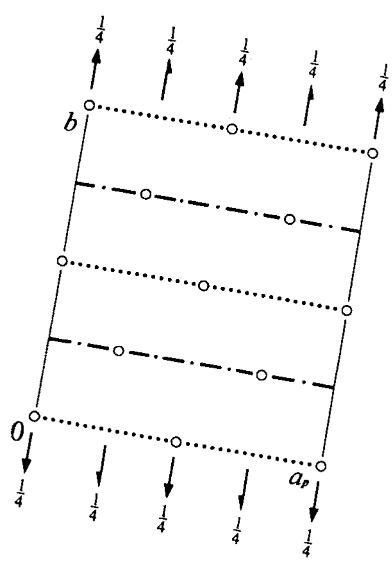
$C2/c$ $\quad$ C_{2h}^{6} $\quad$ $2/m$ $\quad$ Monoclinic

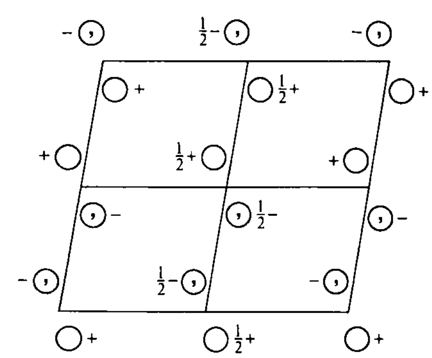
No. 15 $\quad$ $C\,1\,2/c\,1$ $\quad$ Patterson symmetry $C\,1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1









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

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

Symmetry operations

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

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

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

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\quad$ (2) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$ $\quad$ (3) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$ $\quad$ (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	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 : $h+k=2n$ $h0l$: $h,l=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			hkl : $k+l=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $k+l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
4	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			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

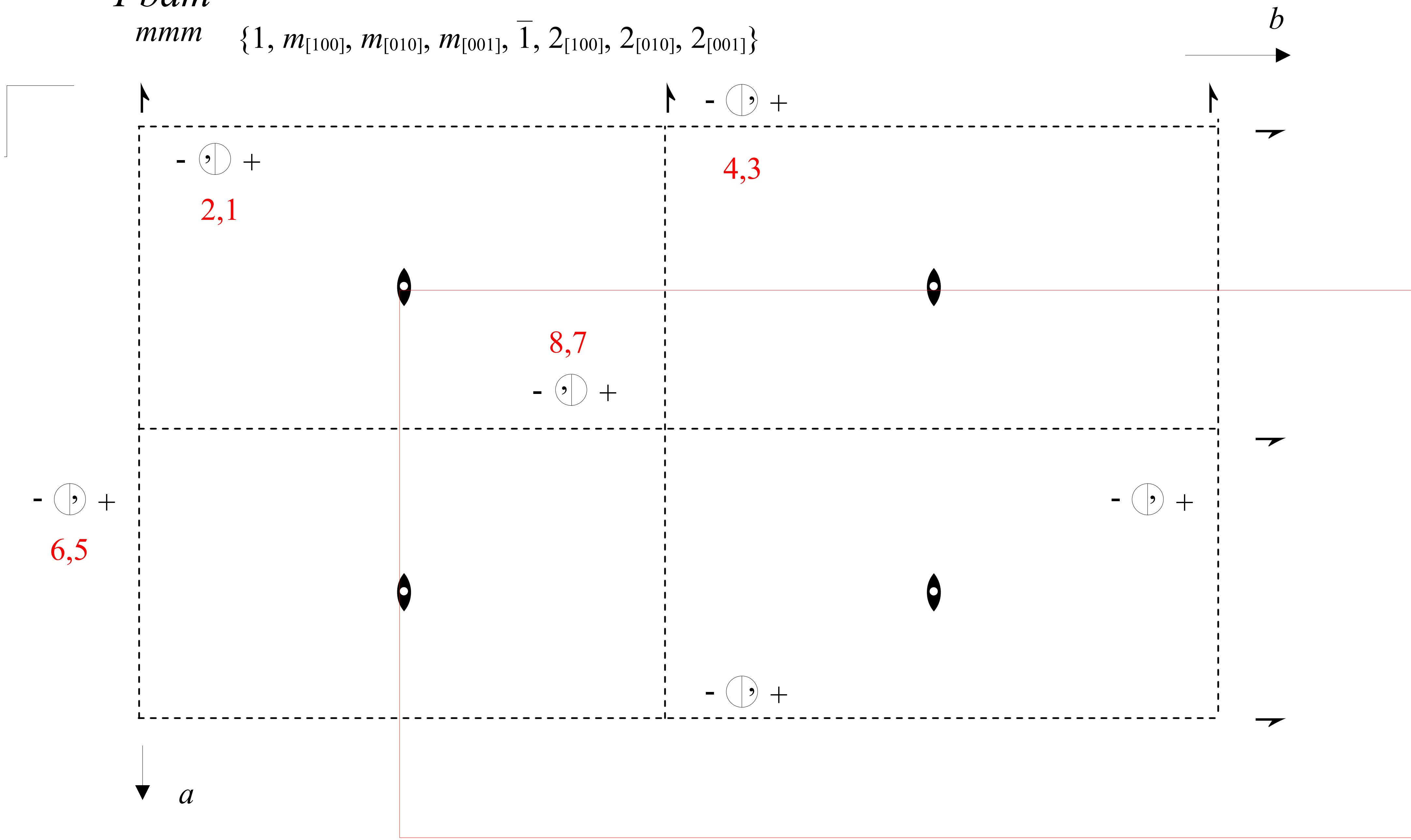
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_1/a$ (88); [3] $P\bar{3}1c$ (163); [3] $P\bar{3}c1$ (165); [3] $R\bar{3}c$ (167)

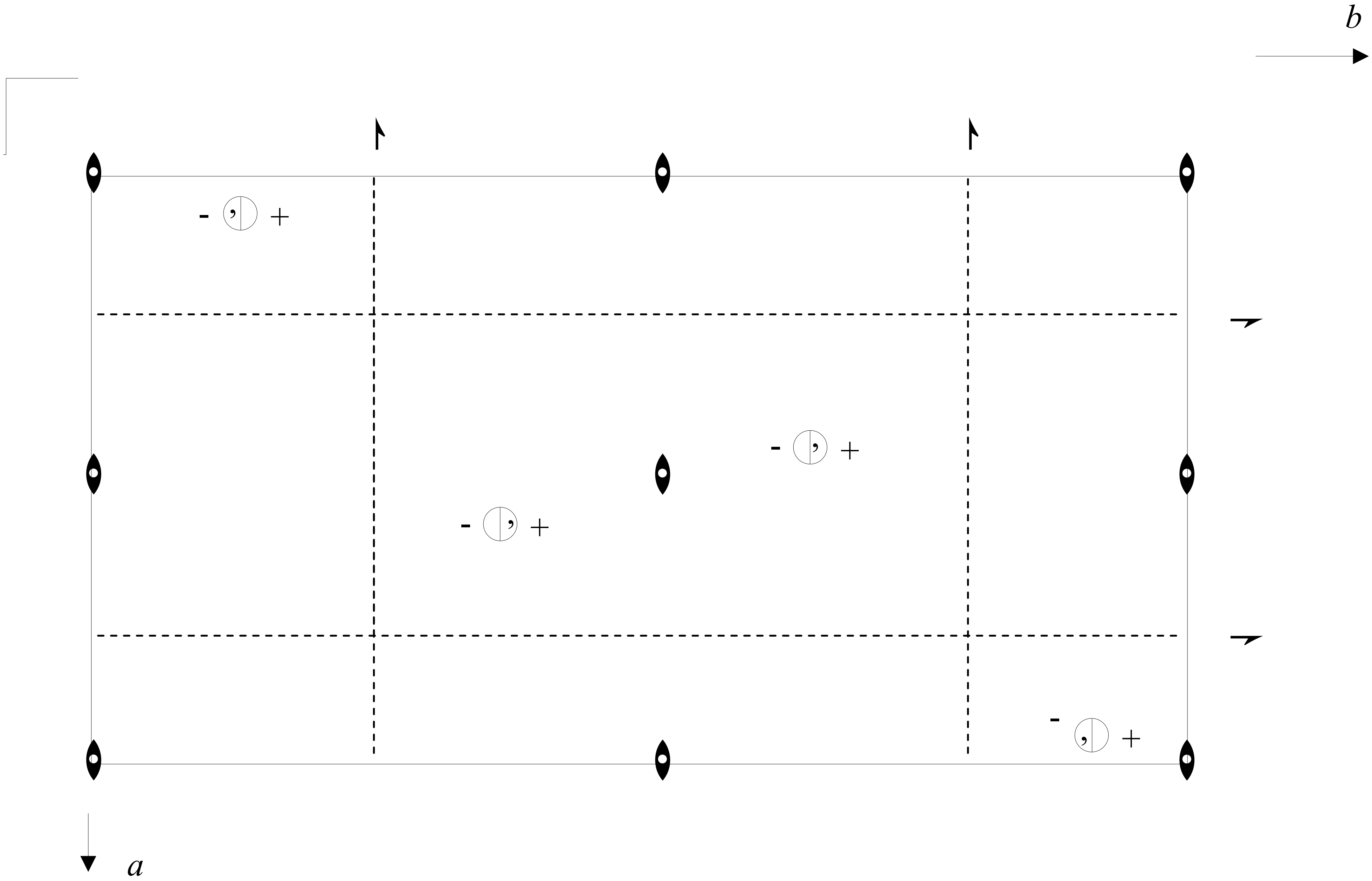
II [2] $F12/m1$ ($C2/m$, 12); [2] $C12/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($C2/m$, 12); [2] $P12/c1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

[100] [010] [001]

Pbam

mmm $\{1, m_{[100]}, m_{[010]}, m_{[001]}, \bar{1}, 2_{[100]}, 2_{[010]}, 2_{[001]}\}$





b
a
- +
- +
- +
- +

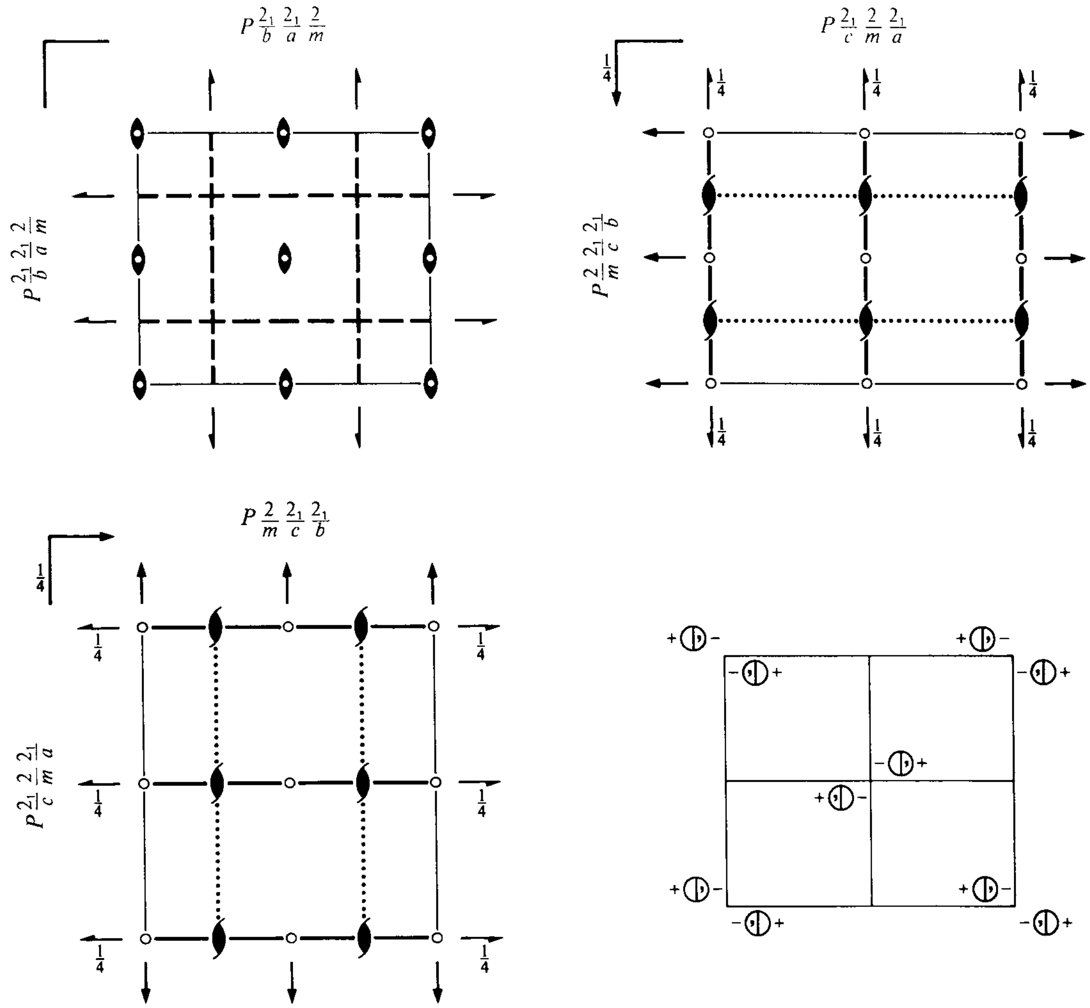
Multiplicity	Site-symmetry group	Coordinates
8	1	$xyz,\ xy\bar{z},\ \tfrac{1}{2}+x,\tfrac{1}{2}-yz,\ \tfrac{1}{2}+x\tfrac{1}{2}-y\bar{z},\ \overline{xyz},\ \overline{xy}z,\ \tfrac{1}{2}-x\tfrac{1}{2}+y\bar{z},\ \tfrac{1}{2}-x\tfrac{1}{2}+yz$
4	$..m$	$xy0,\ \tfrac{1}{2}+x,\tfrac{1}{2}-y0,\ \overline{xy}0,\ \tfrac{1}{2}-x\tfrac{1}{2}+y0$
4	$..m$	$xy\tfrac{1}{2},\ \tfrac{1}{2}+x,\tfrac{1}{2}-y\tfrac{1}{2},\ \overline{xy}\tfrac{1}{2},\ \tfrac{1}{2}-x\tfrac{1}{2}+y\tfrac{1}{2}$
4	$..2$	$00z, 00\bar{z},\ \tfrac{1}{2}\tfrac{1}{2}z, \tfrac{1}{2}\tfrac{1}{2}\bar{z}$
4	$..2$	$\tfrac{1}{2}0z, \tfrac{1}{2}0\bar{z},\ 0\tfrac{1}{2}z,\ 0\tfrac{1}{2}\bar{z}$
2	$..2/m$	$000,\ \tfrac{1}{2}\tfrac{1}{2}0$
2	$..2/m$	$00\tfrac{1}{2},\ \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$
2	$..2/m$	$\tfrac{1}{2}00,\ 0\tfrac{1}{2}0$
2	$..2/m$	$\tfrac{1}{2}0\tfrac{1}{2},\ 0\tfrac{1}{2}\tfrac{1}{2}$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ \bar{y} \\ z \end{bmatrix}$$

International Tables for Crystallography (2006). Vol. A, Space group 55, pp. 282–283.

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 $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

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
							General:
8	*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) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*h*	$..m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	*g*	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	no extra conditions
4	*f*	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl : $h+k=2n$
4	*e*	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	*d*	$..2/m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	*c*	$..2/m$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	*b*	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	*a*	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			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)

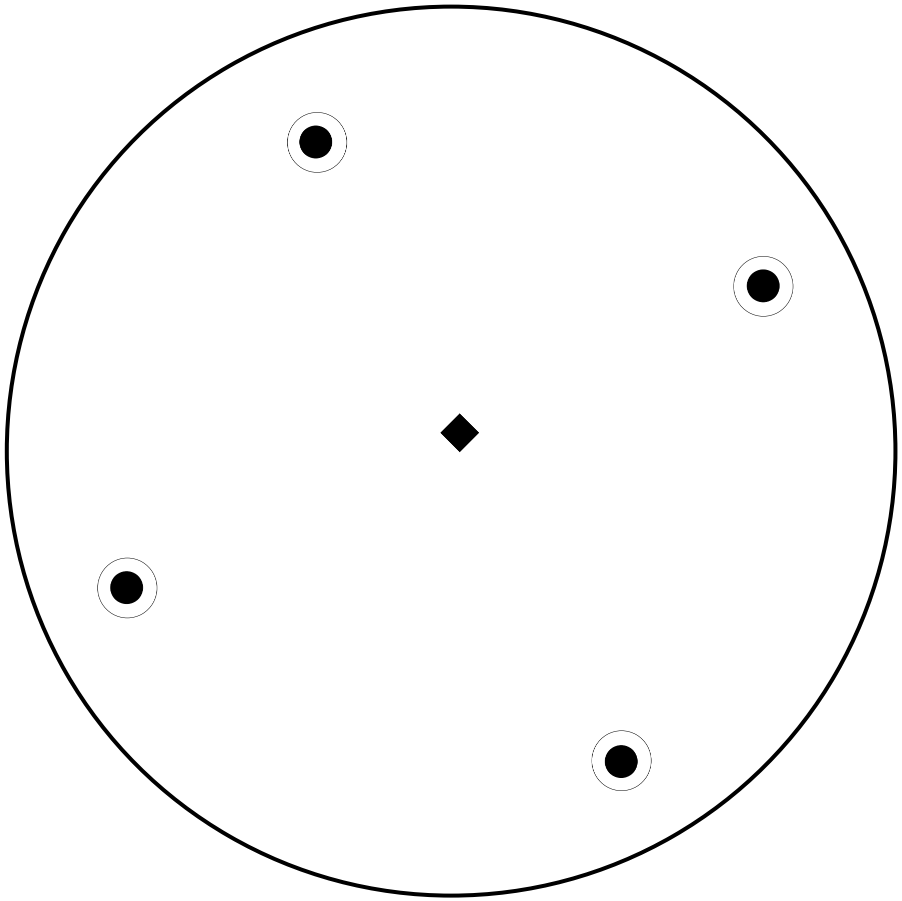
Minimal non-isomorphic supergroups

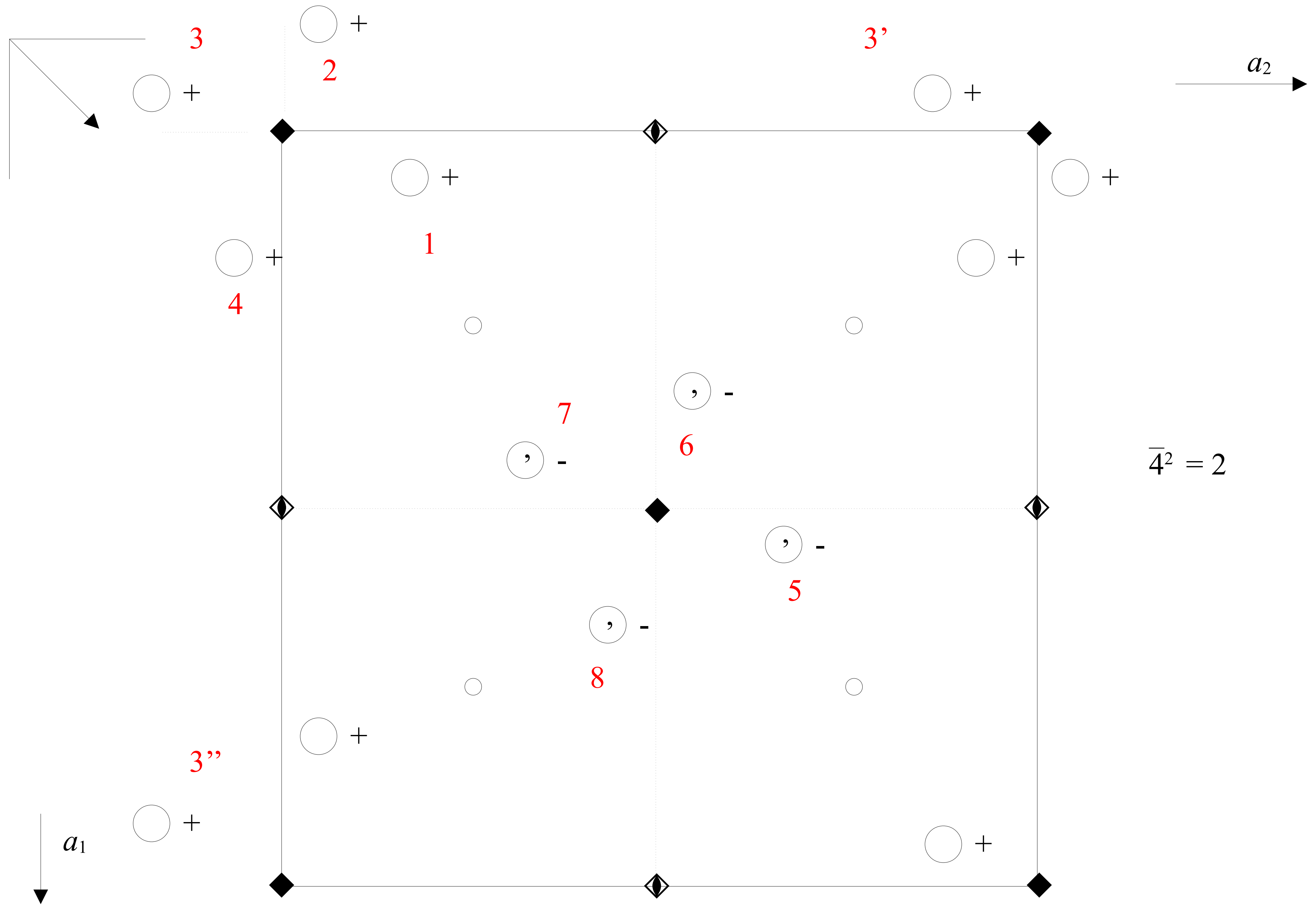
I [2] $P4/mbm$ (127); [2] $P4_2/mbc$ (135)

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)

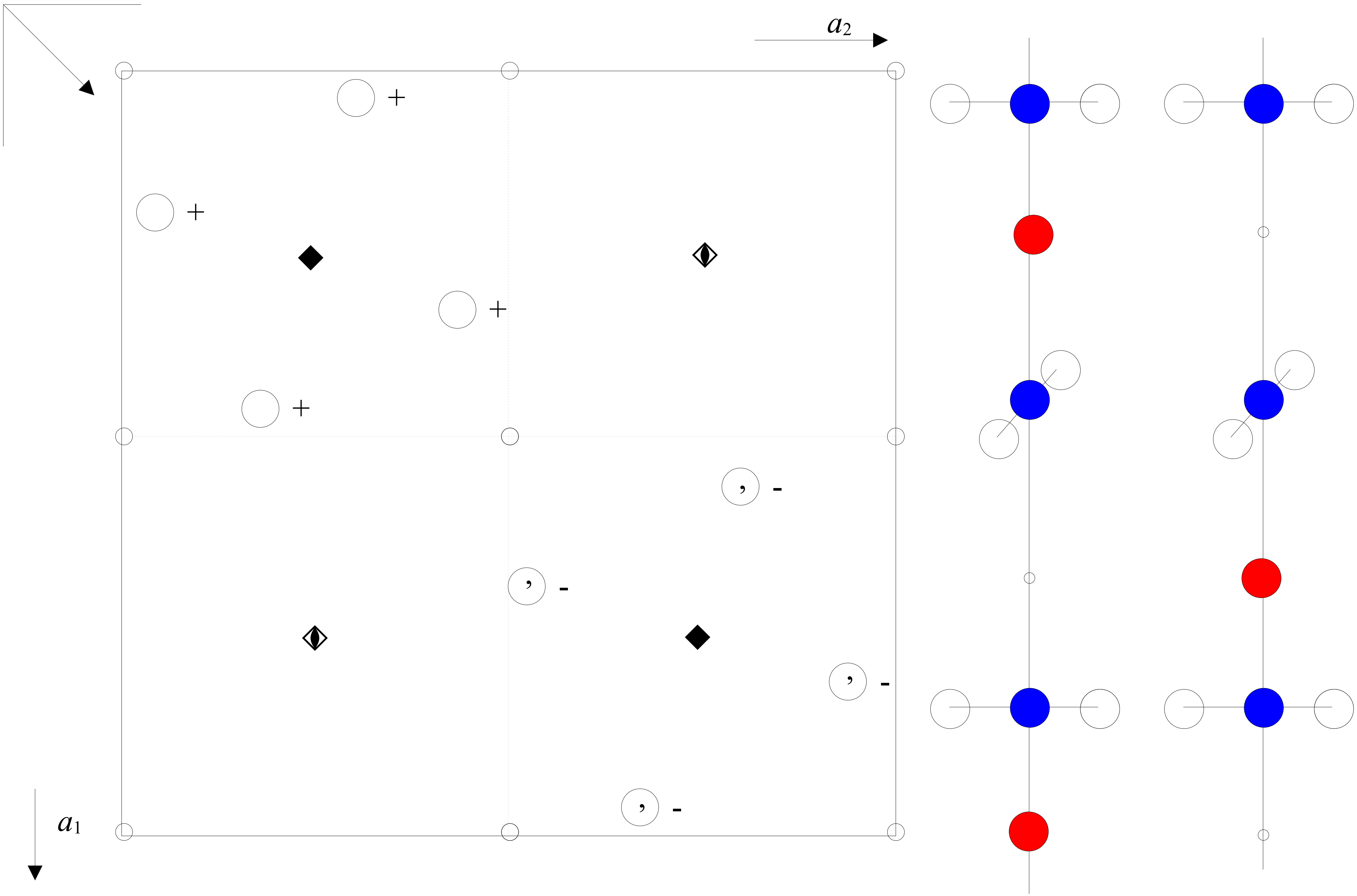
$P4/n \longrightarrow 4/m$

$[001]\ \langle 100 \rangle\ \langle 1\bar{1}0 \rangle$





3
2
3'
a_2
1
4
7
6
$\bar{4}^2 = 2$
5
8
3''
a_1



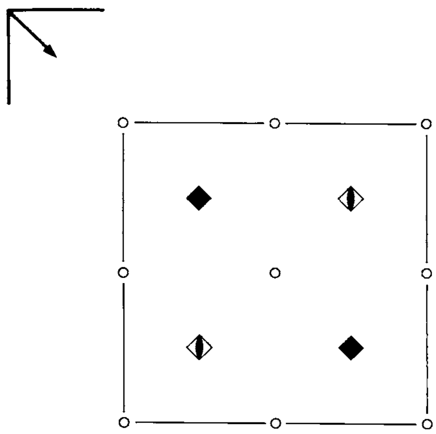
a_2
a_1

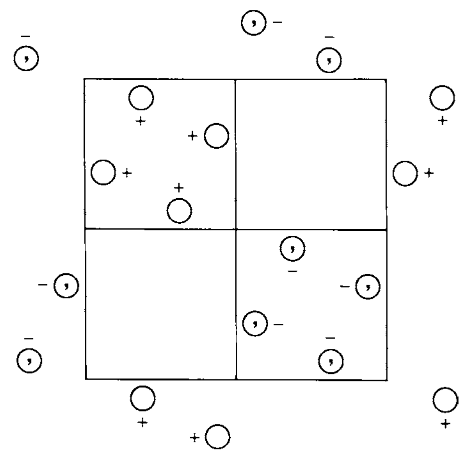
Multiplicity	Site-symmetry group	Coordinates
8	1	$x,y,z;\ y,½-x,z;\ ½-x,½-y,z;\ ½-y,x,z$ $\bar{x},\bar{y},\bar{z};\ \bar{y},½+x,\bar{z};\ ½+x,½+y,\bar{z};\ ½+y,\bar{x},\bar{z}$
2	4..	$¼,¼,z;\ ¾,¾,\bar{z}$
4	2..	$¼,¾,z;\ ¾,¼,z;\ ¾,¼,\bar{z};\ ¼,¾,\bar{z};$
2	$\bar{4}$..	¼,¾,0; ¾,¼,0
2	$\bar{4}$..	¼,¾,½ ; ¾,¼,½
4	$\bar{1}$	000, 0½0, ½½0, ½00
4	$\bar{1}$	00½, 0½½, ½½½, ½0½

$P4/n$ $\quad C_{4h}^{3}$ $\quad 4/m$ $\quad$ Tetragonal

No. 85 $\quad P4/n$ $\quad$ 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 $\quad -\frac{1}{4} \leq x \leq \frac{1}{4}; \quad -\frac{1}{4} \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2 \quad \frac{1}{4},\frac{1}{4},z$	(3) $4^{+} \quad \frac{1}{4},\frac{1}{4},z$	(4) $4^{-} \quad \frac{1}{4},\frac{1}{4},z$
(5) $\bar{1} \quad 0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$	(7) $\bar{4}^{+} \quad \frac{1}{4},-\frac{1}{4},z; \quad \frac{1}{4},-\frac{1}{4},0$	(8) $\bar{4}^{-} \quad -\frac{1}{4},\frac{1}{4},z; \quad -\frac{1}{4},\frac{1}{4},0$

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
							General:
8	*g*	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) $\bar{y},x+\frac{1}{2},\bar{z}$	$hk0$: $h+k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	*f*	$2\,.\,.$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl : $h+k=2n$
4	*e*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h,k=2n$
4	*d*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl : $h,k=2n$
2	*c*	$4\,.\,.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	*b*	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	*a*	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl : $h+k=2n$

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 $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
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] $P2/n$ ($P2/c$, 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)