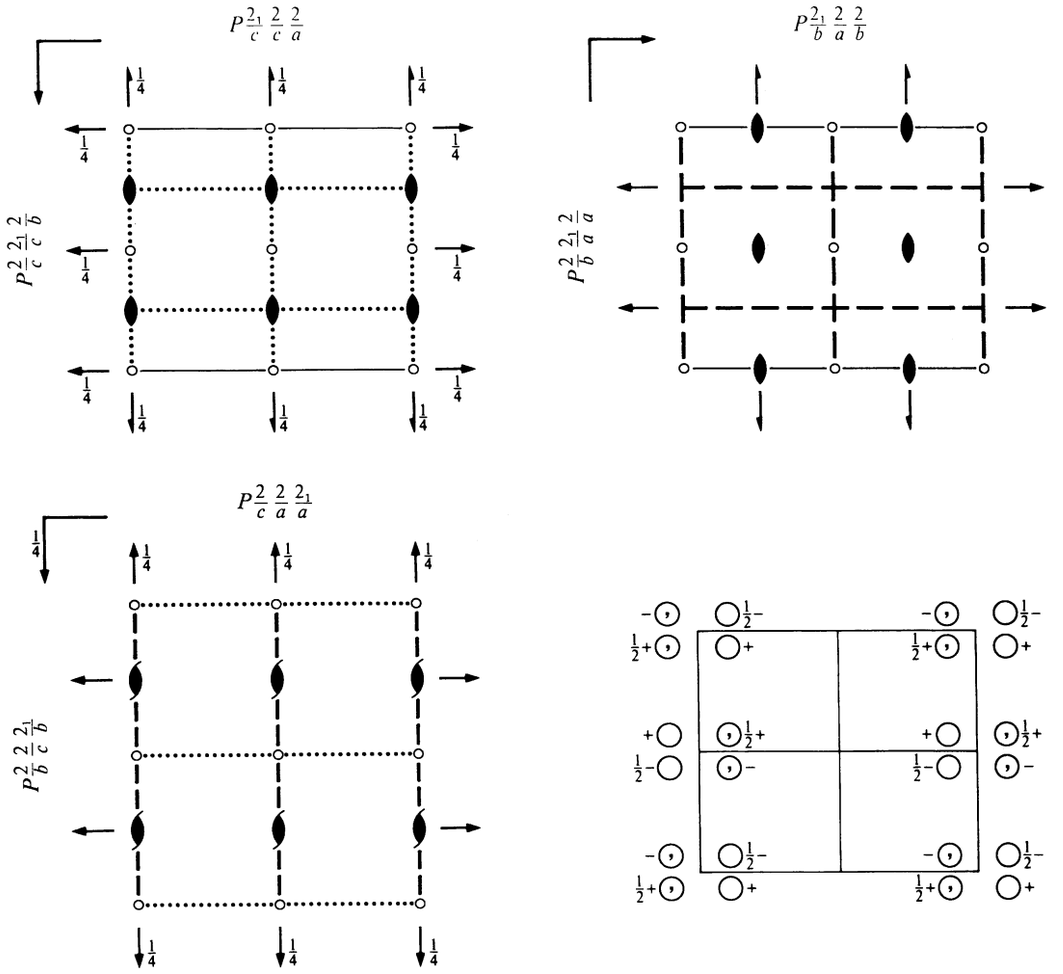
$Pcca$ D_{2h}^{8} mmm Orthorhombic

No. 54 $P\ 2_1/c\ 2/c\ 2/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,c\,a$

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) $2\ \ \frac{1}{4},0,z$ (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) $c\ \ \frac{1}{4},y,z$

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	f	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) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	. . 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	d	. . 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	c	. 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	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h,l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	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)