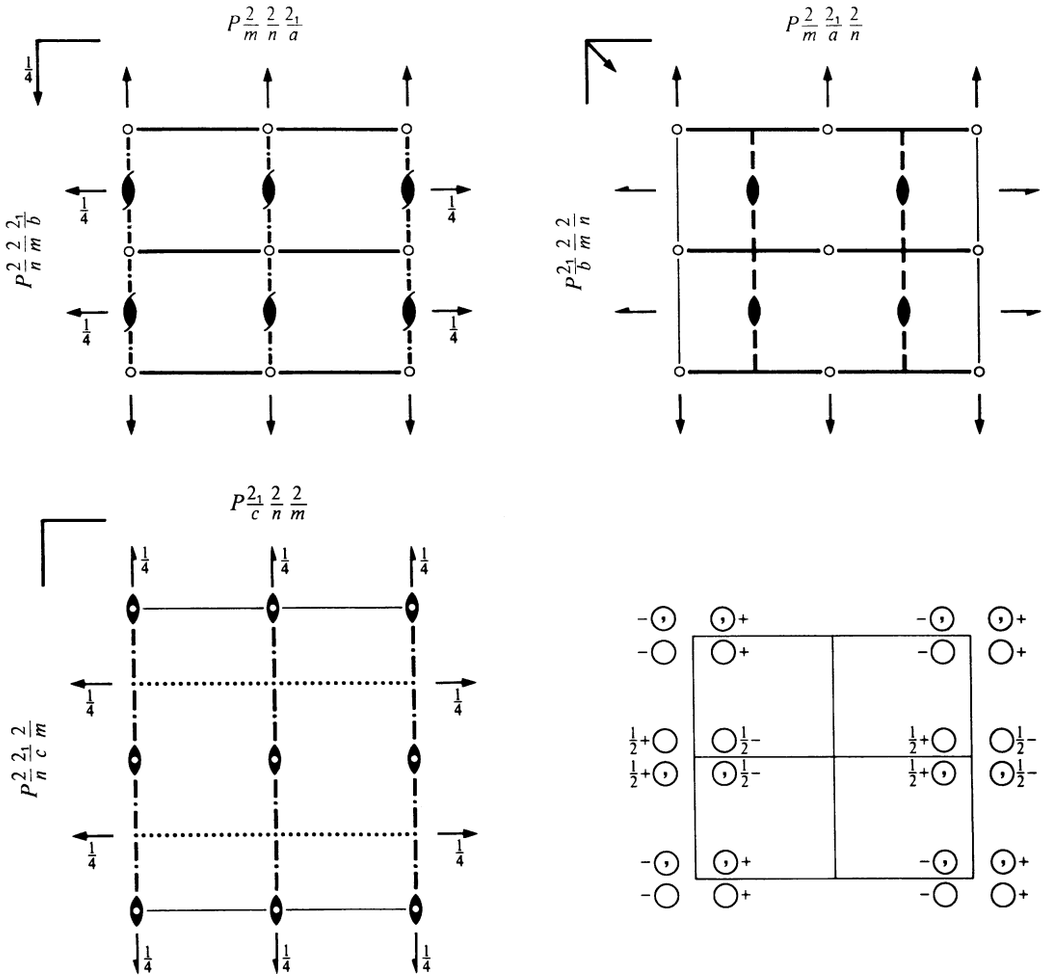
$Pmna$ D_{2h}^{7} mmm Orthorhombic

No. 53 $P\ 2/m\ 2/n\ 2_1/a$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $2/mn1$

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

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) $m\ \ 0,y,z$

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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) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	$h0l$: $h+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*h*	*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	*g*	. 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	*f*	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	*e*	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	*d*	2/*m* . .	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+l=2n$
2	*c*	2/*m* . .	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+l=2n$
2	*b*	2/*m* . .	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl : $h+l=2n$
2	*a*	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] $Pmnn$ ($\mathbf{b}'=2\mathbf{b}$) ($Pnnm$, 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)