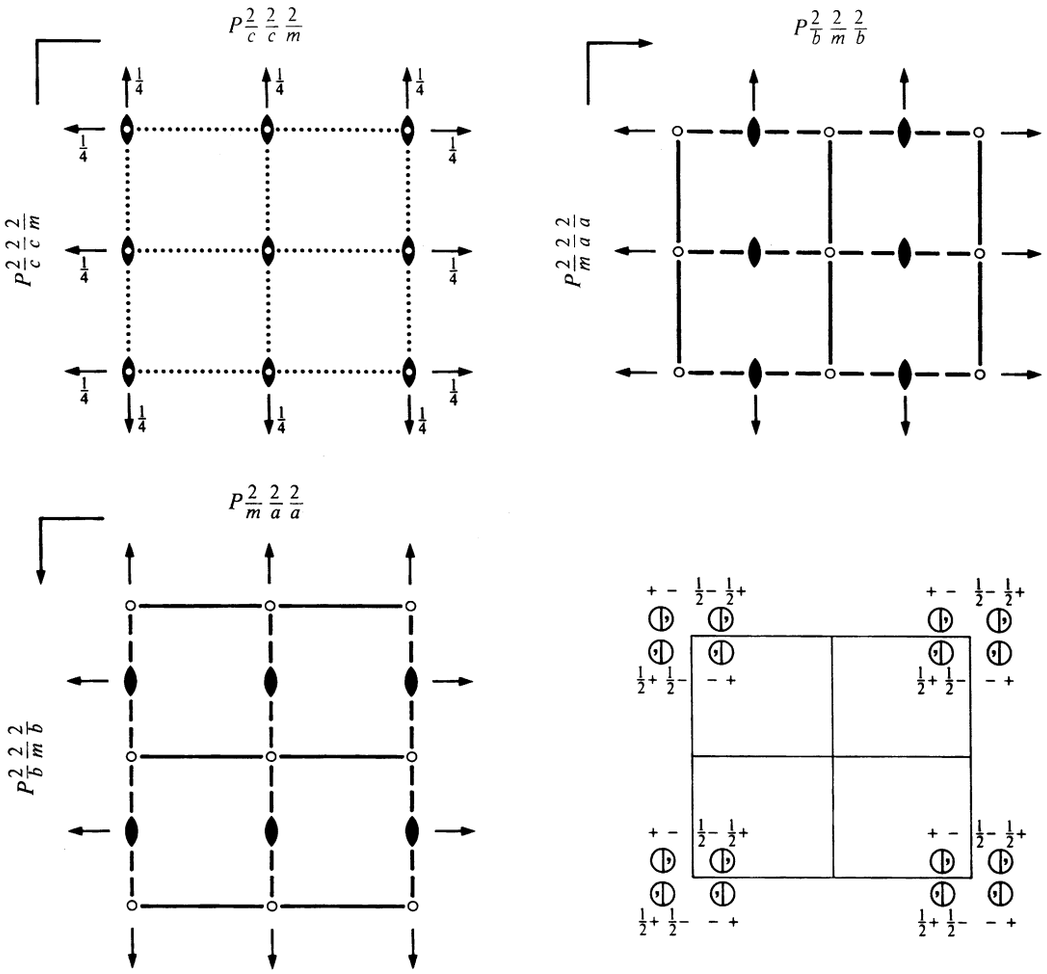
$Pccm$ D_{2h}^3 mmm Orthorhombic

No. 49 $P\ 2/c\ 2/c\ 2/m$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $cc2/m$

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

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,\frac{1}{4}$ (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	r	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) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
4	q	. . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
4	p	. . 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	o	. . 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	n	. . 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	m	. . 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	l	. 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	k	. 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	j	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	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	h	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	g	2 2 2	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	f	2 2 2	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl : $l=2n$
2	e	2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$
2	d	. . 2/m	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $l=2n$
2	c	. . 2/m	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
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] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
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

(*Continued on preceding page*)