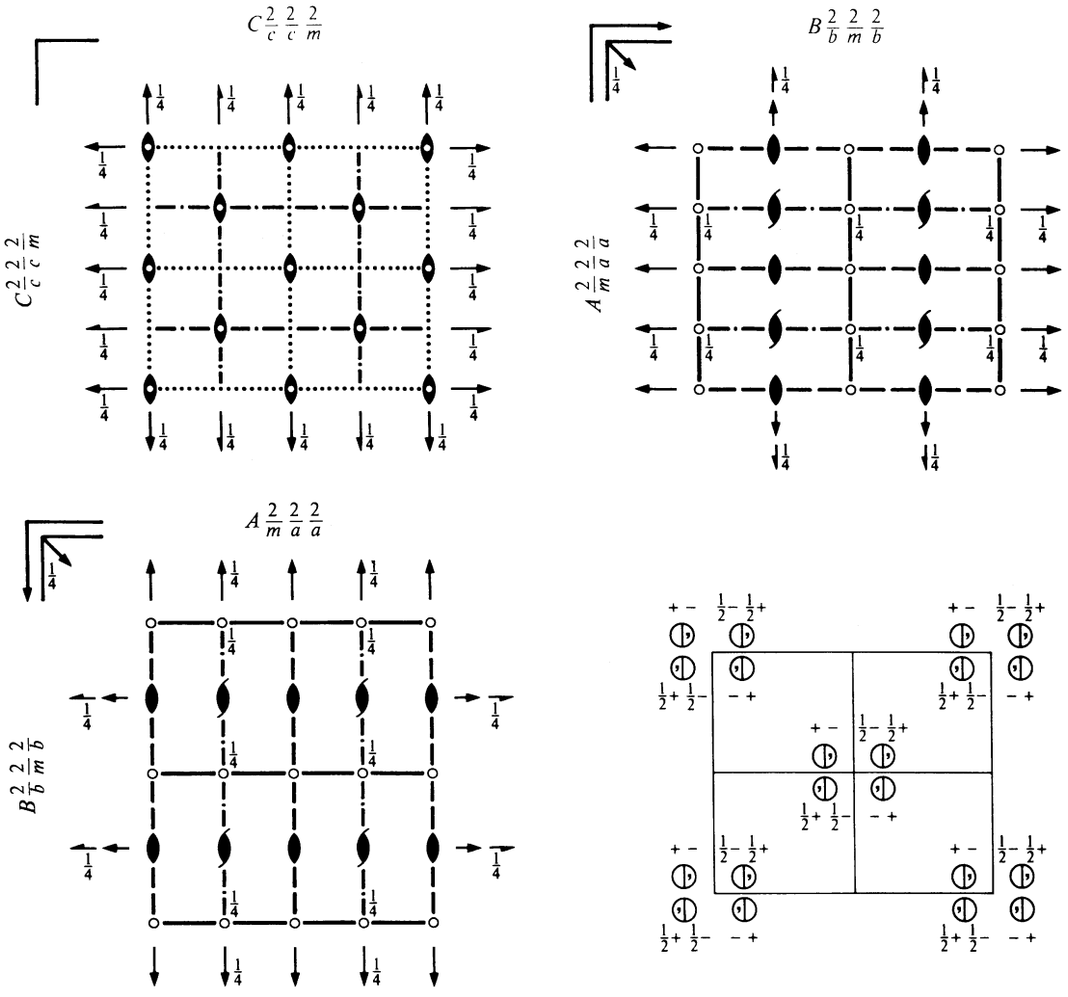
$Cccm$ D_{2h}^{20} mmm Orthorhombic

No. 66 $C\ 2/c\ 2/c\ 2/m$ Patterson symmetry $Cmmm$



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

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

Symmetry operations

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

(1) 1	(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

IIc [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 $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	m	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 : $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $k+l=2n$
8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl : $l=2n$
8	h	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl : $l=2n$
8	g	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl : $l=2n$
4	f	$..2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl : $k+l=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $k+l=2n$
4	d	$..2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
4	c	$..2/m$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
4	b	$2\,2\,2$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
4	a	$2\,2\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			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] $Cc2m$ ($Ama2$, 40)	(1; 3; 6; 8)+
[2] $C2cm$ ($Ama2$, 40)	(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] $C112/m$ ($P2/m$, 10)	(1; 2; 5; 6)+

IIa

[2] $Pnnm$ (58)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pccn$ (56)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pcnm$ ($Pmna$, 53)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pncm$ ($Pmna$, 53)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pncn$ ($Pnna$, 52)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pcnn$ ($Pnna$, 52)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
[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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