

Cmce

D_{2h}^{18}

mmm

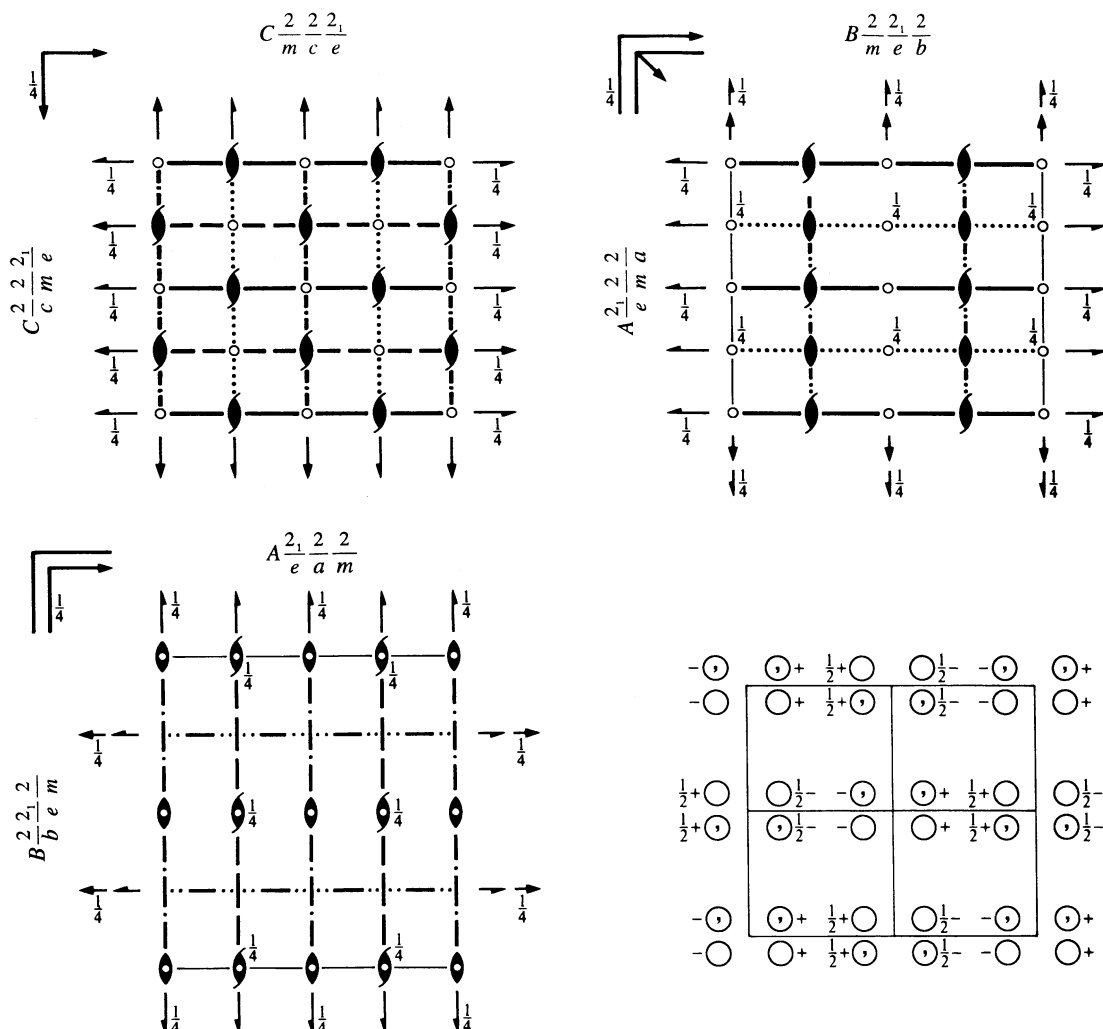
Orthorhombic

No. 64

$C 2/m 2/c 2_1/e$

Patterson symmetry $Cmmm$

Former space-group symbol $Cmca$; cf. Chapter 1.3



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

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

Symmetry operations

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

- | | | | |
|-----------------------|--|--|-----------------|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ | (4) $2 \ x,0,0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) $b \ x,y,\frac{1}{4}$ | (7) $c \ x,\frac{1}{4},z$ | (8) $m \ 0,y,z$ |

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

- | | | | |
|---|--|--|--|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ | (3) $2 \ \frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ | (6) $a \ x,y,\frac{1}{4}$ | (7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$ | (8) $b \ \frac{1}{4},y,z$ |

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); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$				General:
16	<i>g</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) x,\bar{y},\bar{z} (8) \bar{x},y,z	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8	<i>f</i> $m..$	$0,y,z$	$0,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	Special: as above, plus no extra conditions
8	<i>e</i> $.2.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{4}$	$hkl : h=2n$
8	<i>d</i> $2..$	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$	$x,\frac{1}{2},\frac{1}{2}$	$hkl : k+l=2n$
8	<i>c</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$hkl : k,l=2n$
4	<i>b</i> $2/m..$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl : k+l=2n$
4	<i>a</i> $2/m..$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0,0,z

Along [100] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
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] $C2ce$ ($Aea2$, 41)	(1; 4; 6; 7)+
	[2] $Cm2e$ ($Aem2$, 39)	(1; 3; 6; 8)+
	[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+
	[2] $C222_1$ (20)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C112_1/e$ ($P2_1/c$, 14)	(1; 2; 5; 6)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
IIa	[2] $Pmnb$ ($Pnma$, 62)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbca$ (61)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbna$ ($Pbcn$, 60)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmca$ ($Pbcm$, 57)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbnb$ ($Pccn$, 56)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcb$ ($Pbam$, 55)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pbcb$ ($Pcca$, 54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmce$ ($\mathbf{a}' = 3\mathbf{a}$) (64); [3] $Cmce$ ($\mathbf{b}' = 3\mathbf{b}$) (64); [3] $Cmce$ ($\mathbf{c}' = 3\mathbf{c}$) (64)

Minimal non-isomorphic supergroups

I none

II [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmme$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)