

*Cmme*

$D_{2h}^{21}$

*mmm*

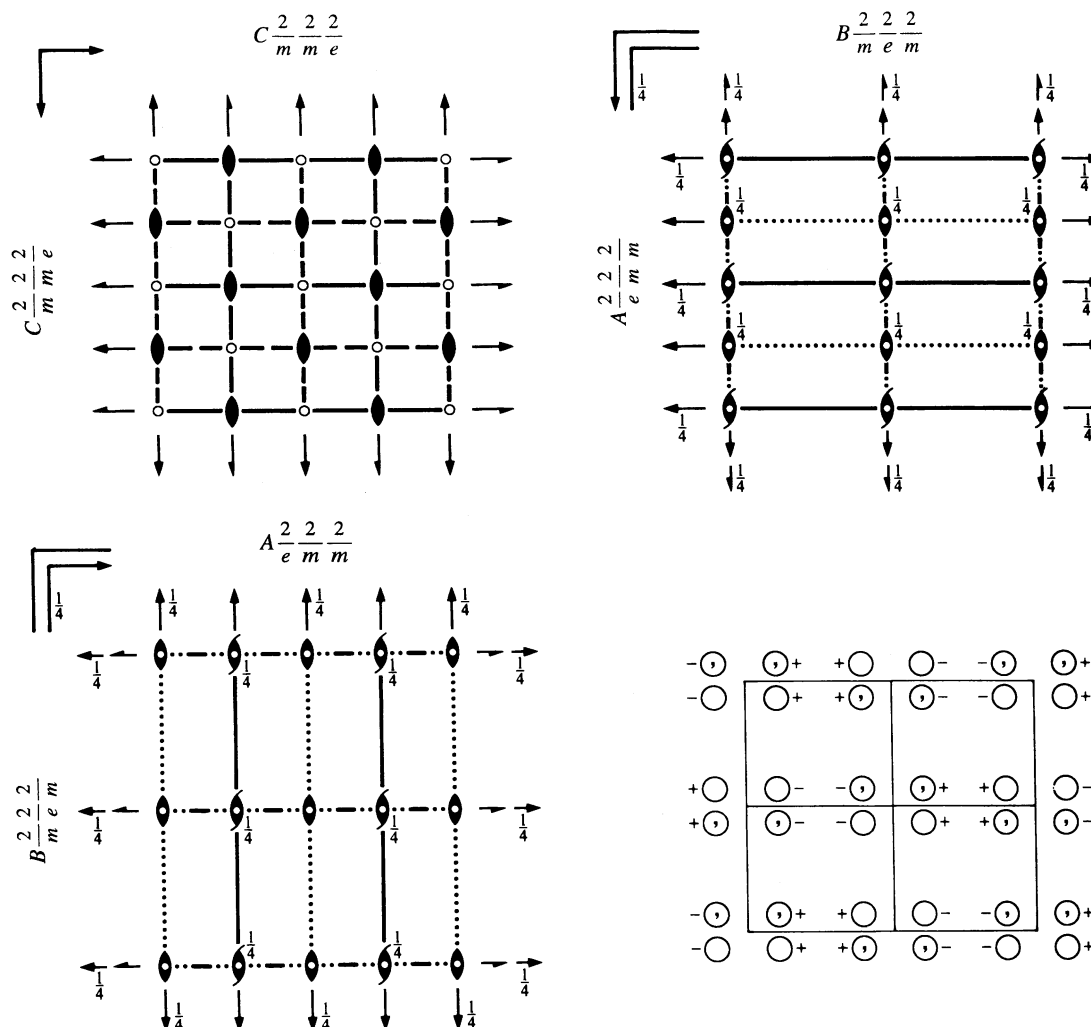
Orthorhombic

No. 67

$C 2/m 2/m 2/e$

Patterson symmetry *Cmmm*

Former space-group symbol *Cmma*; cf. Chapter 1.3



Origin at centre ( $2/m$ ) at  $2/m2_1/e$

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

**Symmetry operations**

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

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

**Maximal isomorphic subgroups of lowest index**

**IIc** [2] *Cmme* ( $c' = 2c$ ) (67); [3] *Cmme* ( $a' = 3a$  or  $b' = 3b$ ) (67)

**Minimal non-isomorphic supergroups**

**I** [2] *P4/nbm* (125); [2] *P4/nmm* (129); [2] *P4<sub>2</sub>/nnm* (134); [2] *P4<sub>2</sub>/ncm* (138)

**II** [2] *Fmmm* (69); [2] *Pmmm* ( $a' = \frac{1}{2}a, b' = \frac{1}{2}b$ ) (47)

**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 o 1	(1) $x,y,z$ (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	$hkl : h+k=2n$ $0kl : k=2n$ $h0l : h=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ Special: as above, plus
8 n .m.	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$	no extra conditions
8 m m..	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8 l ..2	$\frac{1}{4},0,z$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},\frac{1}{2},z$	$hkl : h=2n$
8 k .2.	$\frac{1}{4},y,\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{2}$	$hkl : h=2n$
8 j .2.	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{1}{4},y+\frac{1}{2},0$	$hkl : h=2n$
8 i 2..	$x,0,\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$x,\frac{1}{2},\frac{1}{2}$	$hkl : h=2n$
8 h 2..	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$	$hkl : h=2n$
4 g mm2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4 f .2/m.	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl : h=2n$
4 e .2/m.	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			$hkl : h=2n$
4 d 2/m..	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : h=2n$
4 c 2/m..	$0,0,0$	$0,\frac{1}{2},0$			$hkl : h=2n$
4 b 222	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$			$hkl : h=2n$
4 a 222	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$			$hkl : h=2n$

**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]  $p2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$   $\mathbf{b}' = \mathbf{c}$   
Origin at x,0,0

Along [010]  $p2mm$   
 $\mathbf{a}' = \mathbf{c}$   $\mathbf{b}' = \frac{1}{2}\mathbf{a}$   
Origin at 0,y,0

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $Cm2e$ ( $Aem2$ , 39)	(1; 3; 6; 8)+	<b>IIa</b>	[2] $Pbma$ ( $Pbcm$ , 57)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C2me$ ( $Aem2$ , 39)	(1; 4; 6; 7)+		[2] $Pmab$ ( $Pbcm$ , 57)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Cmm2$ (35)	(1; 2; 7; 8)+		[2] $Pbaa$ ( $Pcca$ , 54)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C222$ (21)	(1; 2; 3; 4)+		[2] $Pbab$ ( $Pcca$ , 54)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C112/e$ ( $P2/c$ , 13)	(1; 2; 5; 6)+		[2] $Pmmb$ ( $Pmma$ , 51)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $C12/m1$ ( $C2/m$ , 12)	(1; 3; 5; 7)+		[2] $Pmma$ (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C2/m11$ ( $C2/m$ , 12)	(1; 4; 5; 8)+		[2] $Pmaa$ ( $Pccm$ , 49)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
				[2] $Pbmb$ ( $Pccm$ , 49)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
<b>IIb</b>	[2] $Ccce$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (68); [2] $Ccme$ ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $Cmce$ , 64); [2] $Cmce$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (64); [2] $Imma$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (74); [2] $Ibca$ ( $\mathbf{c}' = 2\mathbf{c}$ ) (73); [2] $Ibmb$ ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $Ibam$ , 72); [2] $Imaa$ ( $\mathbf{c}' = 2\mathbf{c}$ ) ( $Ibam$ , 72)				

(Continued on preceding page)