

$Cmmm$

$D_{2h}^{19}$

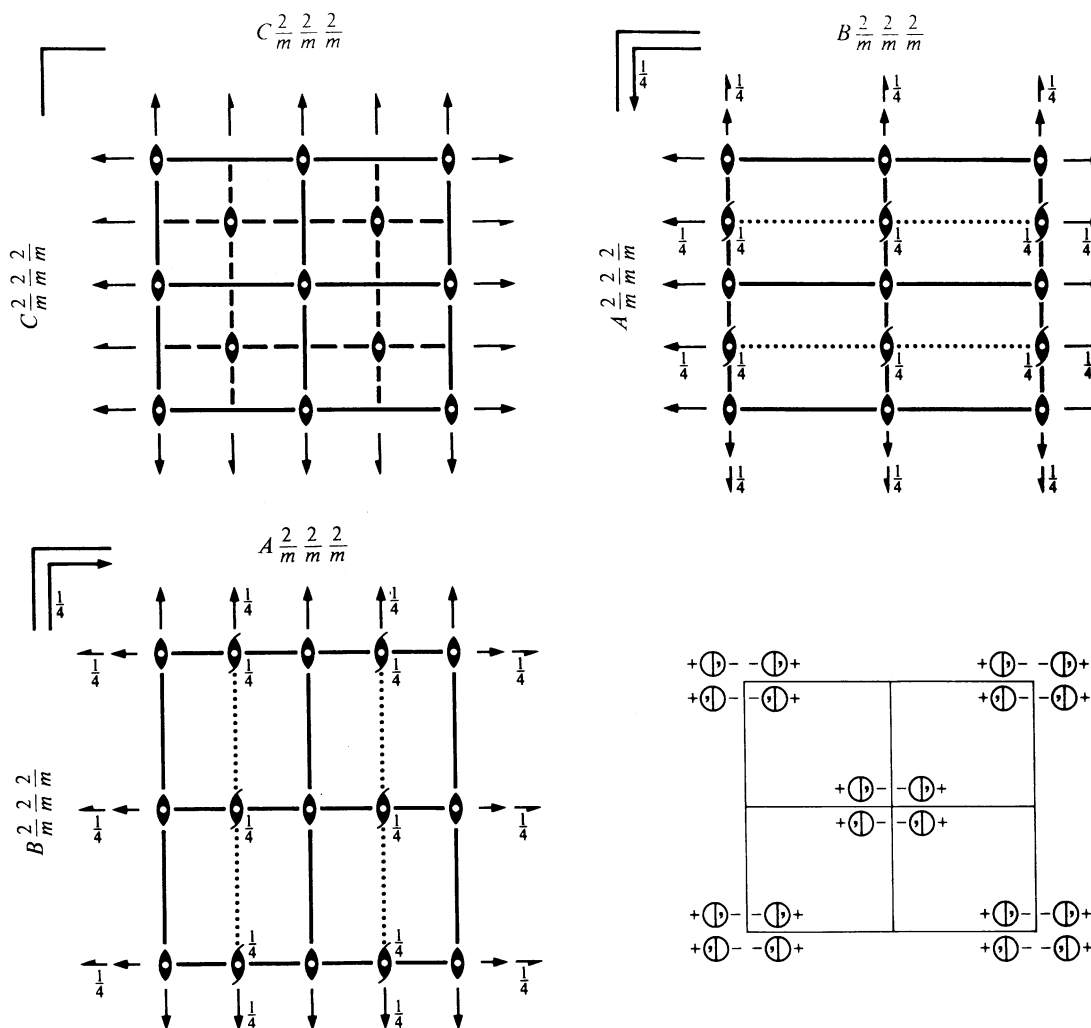
$mmm$

Orthorhombic

No. 65

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

Patterson symmetry  $Cmmm$



Origin at centre ( $mmm$ )

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

**Symmetry of special projections**

Along [001] *c2mm*  
 $\mathbf{a}' = \mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
 Origin at 0,0,z

Along [100] *p2mm*  
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \mathbf{c}$   
 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**

- I** [2] *Cm2m* (*Amm2*, 38) (1; 3; 6; 8)+  
 [2] *C2mm* (*Amm2*, 38) (1; 4; 6; 7)+  
 [2] *Cmm2* (35) (1; 2; 7; 8)+  
 [2] *C222* (21) (1; 2; 3; 4)+  
 [2] *C12/m1* (*C2/m*, 12) (1; 3; 5; 7)+  
 [2] *C2/m11* (*C2/m*, 12) (1; 4; 5; 8)+  
 [2] *C112/m* (*P2/m*, 10) (1; 2; 5; 6)+
- IIa** [2] *Pmmn* (59) 1; 2; 7; 8; (3; 4; 5; 6) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pbam* (55) 1; 2; 5; 6; (3; 4; 7; 8) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pbmn* (*Pmna*, 53) 1; 3; 5; 7; (2; 4; 6; 8) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pman* (*Pmna*, 53) 1; 4; 5; 8; (2; 3; 6; 7) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pmam* (*Pmma*, 51) 1; 3; 6; 8; (2; 4; 5; 7) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pbmm* (*Pmma*, 51) 1; 4; 6; 7; (2; 3; 5; 8) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pban* (50) 1; 2; 3; 4; (5; 6; 7; 8) +  $(\frac{1}{2}, \frac{1}{2}, 0)$   
 [2] *Pmmm* (47) 1; 2; 3; 4; 5; 6; 7; 8
- IIb** [2] *Cccm* ( $\mathbf{c}' = 2\mathbf{c}$ ) (66); [2] *Ccmm* ( $\mathbf{c}' = 2\mathbf{c}$ ) (*Cmcm*, 63); [2] *Cmcm* ( $\mathbf{c}' = 2\mathbf{c}$ ) (63); [2] *Ibmm* ( $\mathbf{c}' = 2\mathbf{c}$ ) (*Imma*, 74);  
 [2] *Imam* ( $\mathbf{c}' = 2\mathbf{c}$ ) (*Imma*, 74); [2] *Ibam* ( $\mathbf{c}' = 2\mathbf{c}$ ) (72); [2] *Immm* ( $\mathbf{c}' = 2\mathbf{c}$ ) (71)

**Maximal isomorphic subgroups of lowest index**

- IIc** [2] *Cmmm* ( $\mathbf{c}' = 2\mathbf{c}$ ) (65); [3] *Cmmm* ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$ ) (65)

**Minimal non-isomorphic supergroups**

- I** [2] *P4/mmm* (123); [2] *P4/mbm* (127); [2] *P4/mcm* (132); [2] *P4<sub>2</sub>/mnm* (136); [3] *P6/mmm* (191)
- II** [2] *Fmmm* (69); [2] *Pmmm* ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ,  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) (47)