

I m m m

D_{2h}^{25}

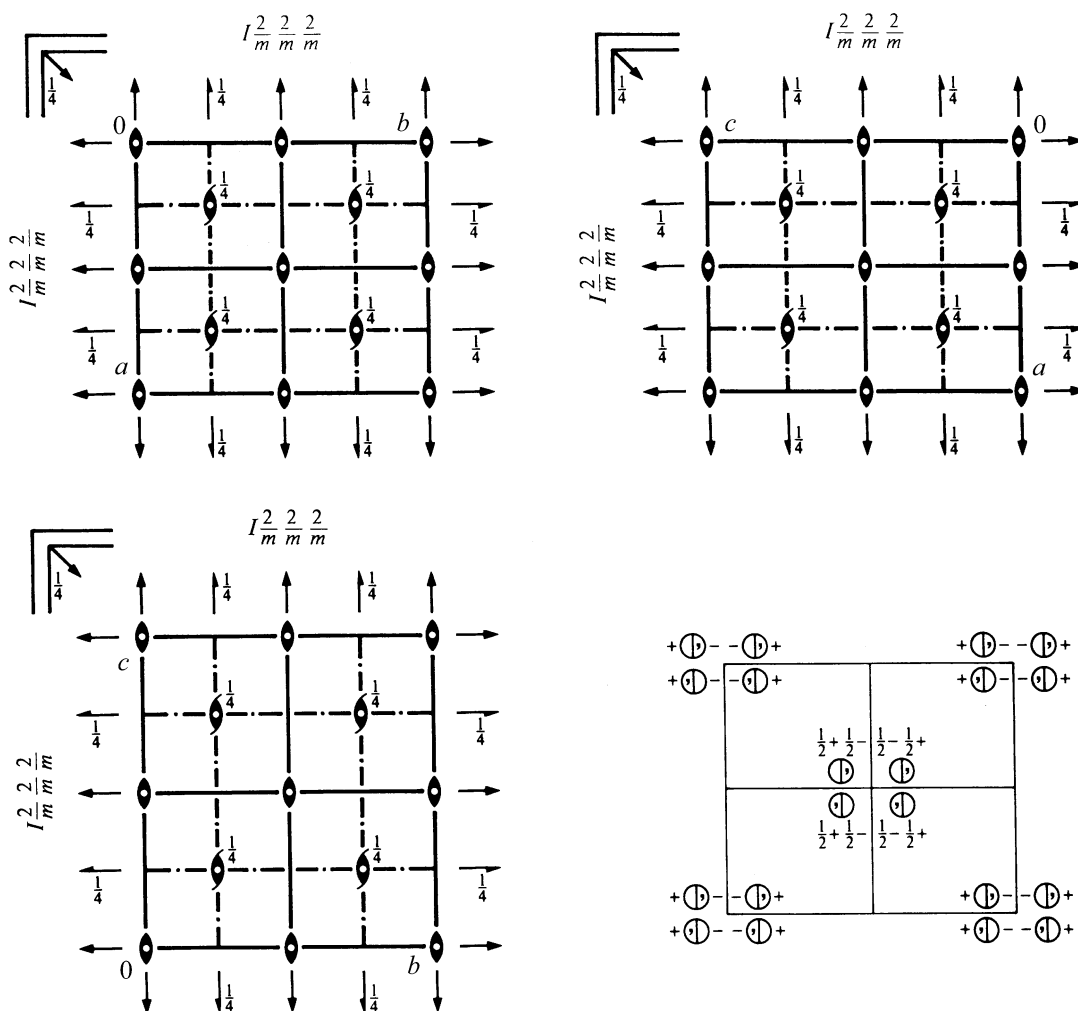
m m m

Orthorhombic

No. 71

I 2/m 2/m 2/m

Patterson symmetry *I m m m*



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

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

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

Symmetry of special projections

Along [001] *c* 2 *m m*
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] *c* 2 *m m*
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

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