

$Cmcm$

D_{2h}^{17}

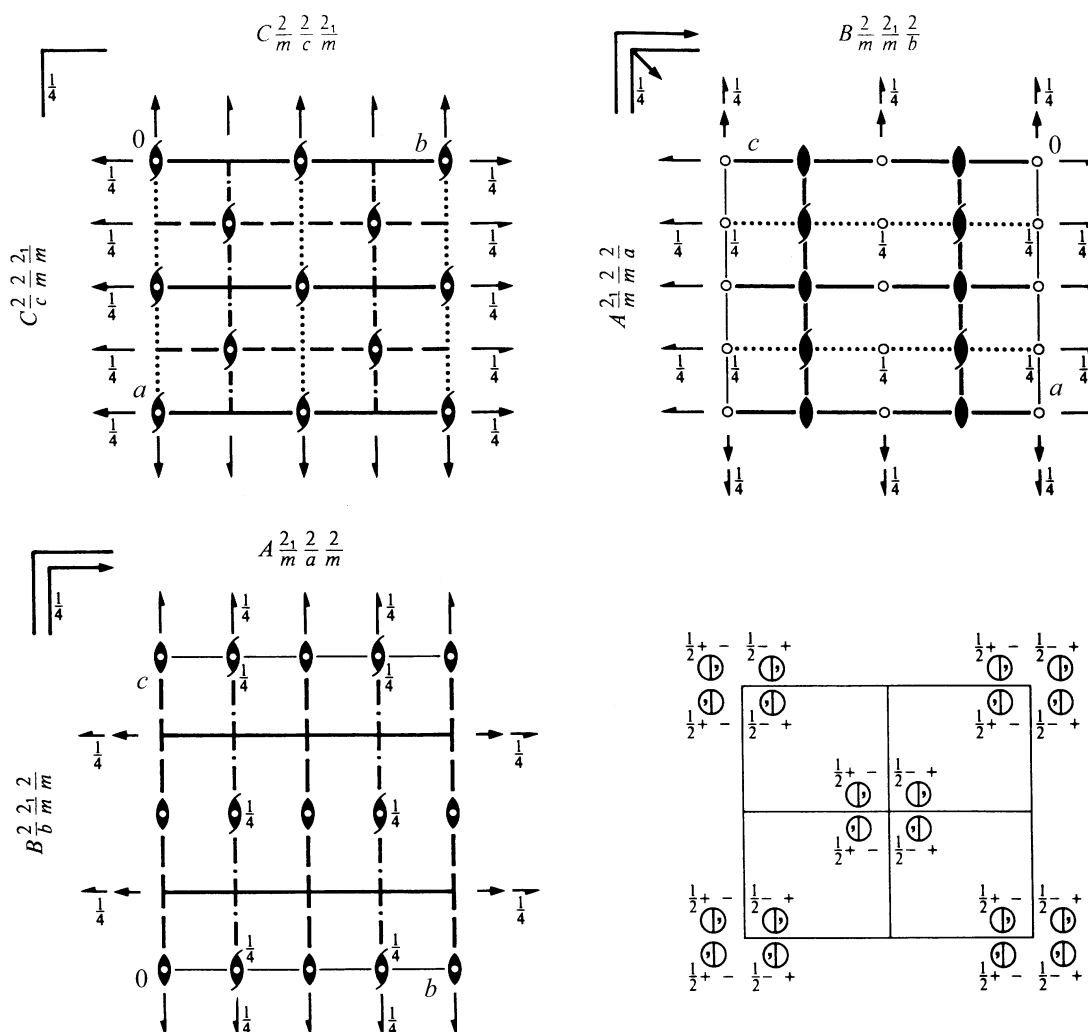
mmm

Orthorhombic

No. 63

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

Patterson symmetry $Cmcm$



Origin at centre ($2/m$) at $2/mc2_1$

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

Symmetry operations

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

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

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

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

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

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

Reflection conditions

General:

16 *h* 1 (1) x, y, z (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (4) x, \bar{y}, \bar{z}
(5) $\bar{x}, \bar{y}, \bar{z}$ (6) $x, y, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y}, z + \frac{1}{2}$ (8) \bar{x}, y, z

$hkl: h + k = 2n$

$0kl: k = 2n$

$h0l: h, l = 2n$

$hk0: h + k = 2n$

$h00: h = 2n$

$0k0: k = 2n$

$00l: l = 2n$

Special: as above, plus

no extra conditions

no extra conditions

$hkl: l = 2n$

$hkl: k, l = 2n$

no extra conditions

$hkl: l = 2n$

$hkl: l = 2n$

8 *g* $..m$ $x, y, \frac{1}{4}$ $\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{x}, y, \frac{1}{4}$ $x, \bar{y}, \frac{3}{4}$
8 *f* $m..$ $0, y, z$ $0, \bar{y}, z + \frac{1}{2}$ $0, y, \bar{z} + \frac{1}{2}$ $0, \bar{y}, \bar{z}$
8 *e* $2..$ $x, 0, 0$ $\bar{x}, 0, \frac{1}{2}$ $\bar{x}, 0, 0$ $x, 0, \frac{1}{2}$
8 *d* $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, 0$
4 *c* $m2m$ $0, y, \frac{1}{4}$ $0, \bar{y}, \frac{3}{4}$
4 *b* $2/m..$ $0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$
4 *a* $2/m..$ $0, 0, 0$ $0, 0, \frac{1}{2}$

Symmetry of special projections

Along $[001]$ $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

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 $0, y, 0$