

Ibam

D_{2h}^{26}

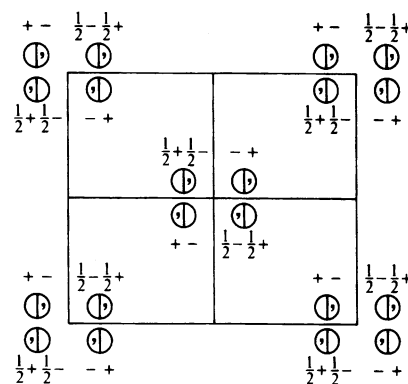
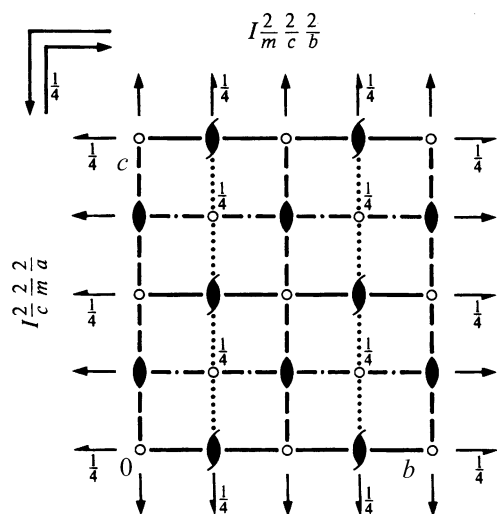
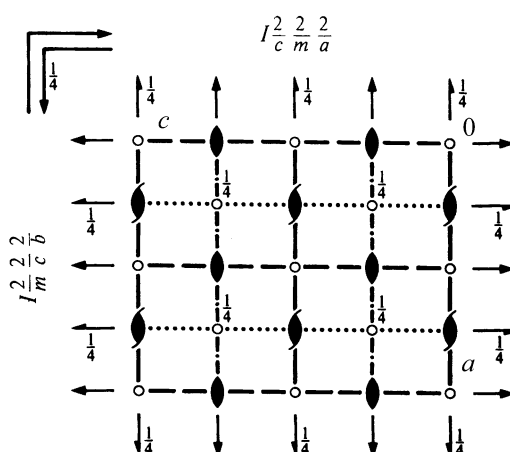
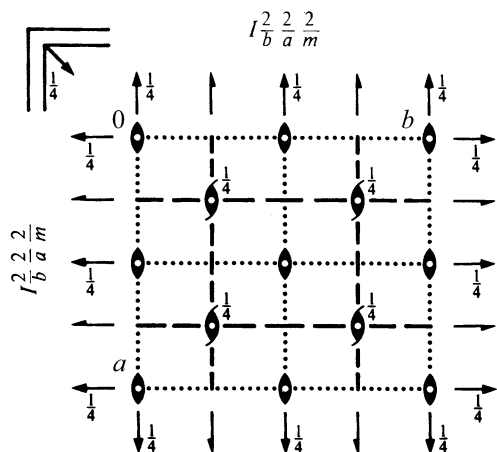
mmm

Orthorhombic

No. 72

I 2/b 2/a 2/m

Patterson symmetry *Immm*



Origin at centre ($2/m$) at $cc2/m$

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

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) $2 \ 0, y, \frac{1}{4}$ | (4) $2 \ x, 0, \frac{1}{4}$ |
| (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) $c \ x, 0, z$ | (8) $c \ 0, y, z$ |

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

General:

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

$hkl: h + k + l = 2n$
 $0kl: k, l = 2n$
 $h0l: h, l = 2n$
 $hk0: h + k = 2n$
 $h00: h = 2n$
 $0k0: k = 2n$
 $00l: l = 2n$

Special: as above, plus

no extra conditions

 $hkl: l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$ $hkl: k, l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$

8 *j* .. *m* $x, y, 0$ $\bar{x}, \bar{y}, 0$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$

8 *i* .. 2 $0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z$

8 *h* .. 2 $0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$

8 *g* . 2. $0, y, \frac{1}{4}$ $0, \bar{y}, \frac{1}{4}$ $0, \bar{y}, \frac{3}{4}$ $0, y, \frac{3}{4}$

8 *f* 2.. $x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$ $x, 0, \frac{3}{4}$

8 *e* $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$

4 *d* .. $2/m$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$

4 *c* .. $2/m$ $0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$

4 *b* 222 $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$

4 *a* 222 $0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$

Symmetry of special projectionsAlong $[001]$ $c2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along $[100]$ $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x, 0, 0$ Along $[010]$ $p2mm$ $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$ Origin at $0, y, 0$