

*Iba*2

C_{2v}^{21}

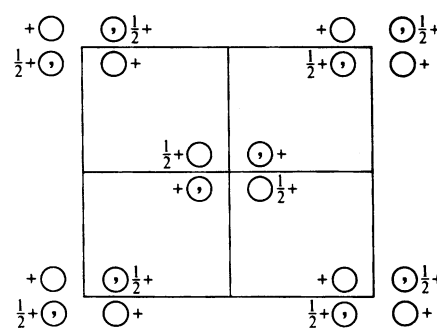
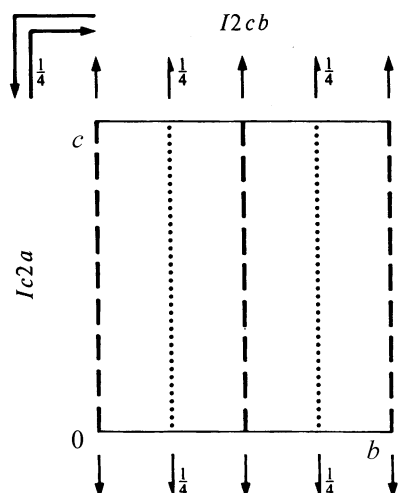
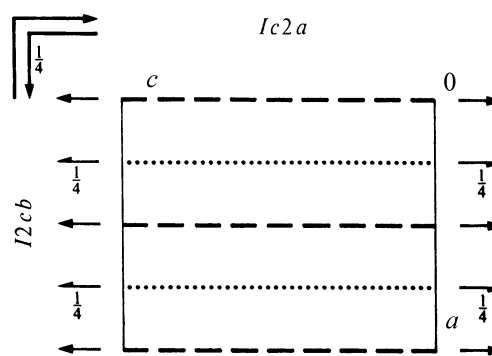
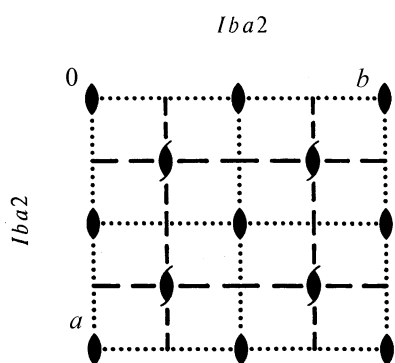
*mm*2

Orthorhombic

No. 45

*Iba*2

Patterson symmetry *Immm*



Origin on *cc*2

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

Symmetry operations

For (0,0,0)+ set

- (1) 1 (2) 2 $0,0,z$ (3) *a* $x, \frac{1}{4}, z$ (4) *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) *c* $x, 0, z$ (4) *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)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

Reflection conditions

General:

8 *c* 1 (1) x, y, z (2) \bar{x}, \bar{y}, z (3) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (4) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$

$hkl: h + k + l = 2n$

$0kl: k, l = 2n$

$h0l: h, l = 2n$

$hk0: h + k = 2n$

$h00: h = 2n$

$0k0: k = 2n$

$00l: l = 2n$

Special: as above, plus

4 *b* .. 2 $0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$

$hkl: l = 2n$

4 *a* .. 2 $0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$

$hkl: l = 2n$

Symmetry of special projections

Along $[001]$ $c2mm$

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

Origin at $0, 0, z$

Along $[100]$ $p1m1$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along $[010]$ $p11m$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$

Origin at $0, y, 0$