

Ibca

D_{2h}^{27}

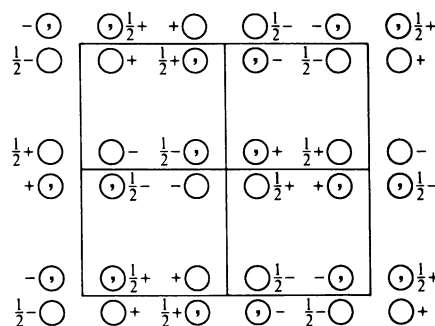
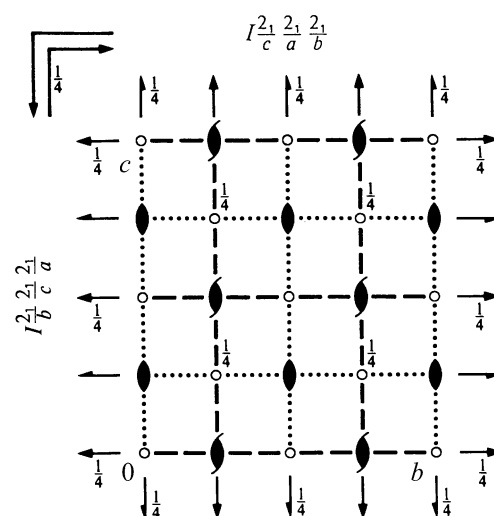
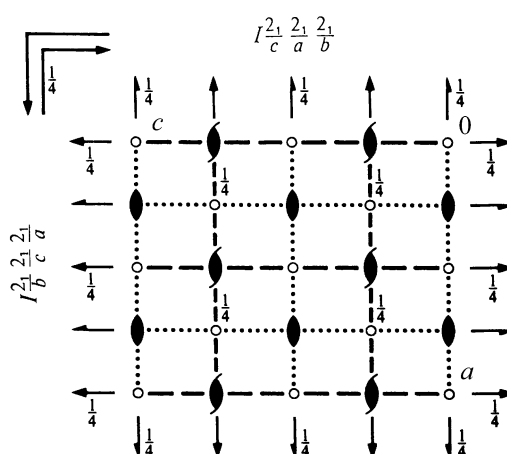
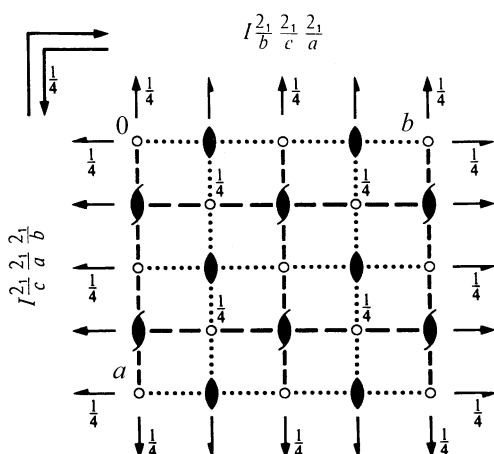
mmm

Orthorhombic

No. 73

$I 2_1/b 2_1/c 2_1/a$

Patterson symmetry *Immm*



Origin at $\bar{1}$ at *cab*

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) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ | (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) <i>a</i> $x,y,\frac{1}{4}$ | (7) <i>c</i> $x,\frac{1}{4},z$ | (8) <i>b</i> $\frac{1}{4},y,z$ |

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

- | | | | |
|---|-------------------------|-------------------------|-------------------------|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) 2 $0,\frac{1}{4},z$ | (3) 2 $\frac{1}{4},y,0$ | (4) 2 $x,0,\frac{1}{4}$ |
| (5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (6) <i>b</i> $x,y,0$ | (7) <i>a</i> $x,0,z$ | (8) <i>c</i> $0,y,z$ |

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

8 *e* .. 2 $0, \frac{1}{4}, z$ $0, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $0, \frac{3}{4}, \bar{z}$ $0, \frac{1}{4}, z + \frac{1}{2}$

$hkl: l = 2n$

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

$hkl: k = 2n$

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

$hkl: h = 2n$

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

$hkl: k, l = 2n$

8 *a* $\bar{1}$ $0, 0, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$

$hkl: k, l = 2n$

Symmetry of special projections

Along [001] $p2mm$

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

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 $0, y, 0$