

Cmce

D_{2h}^{18}

mmm

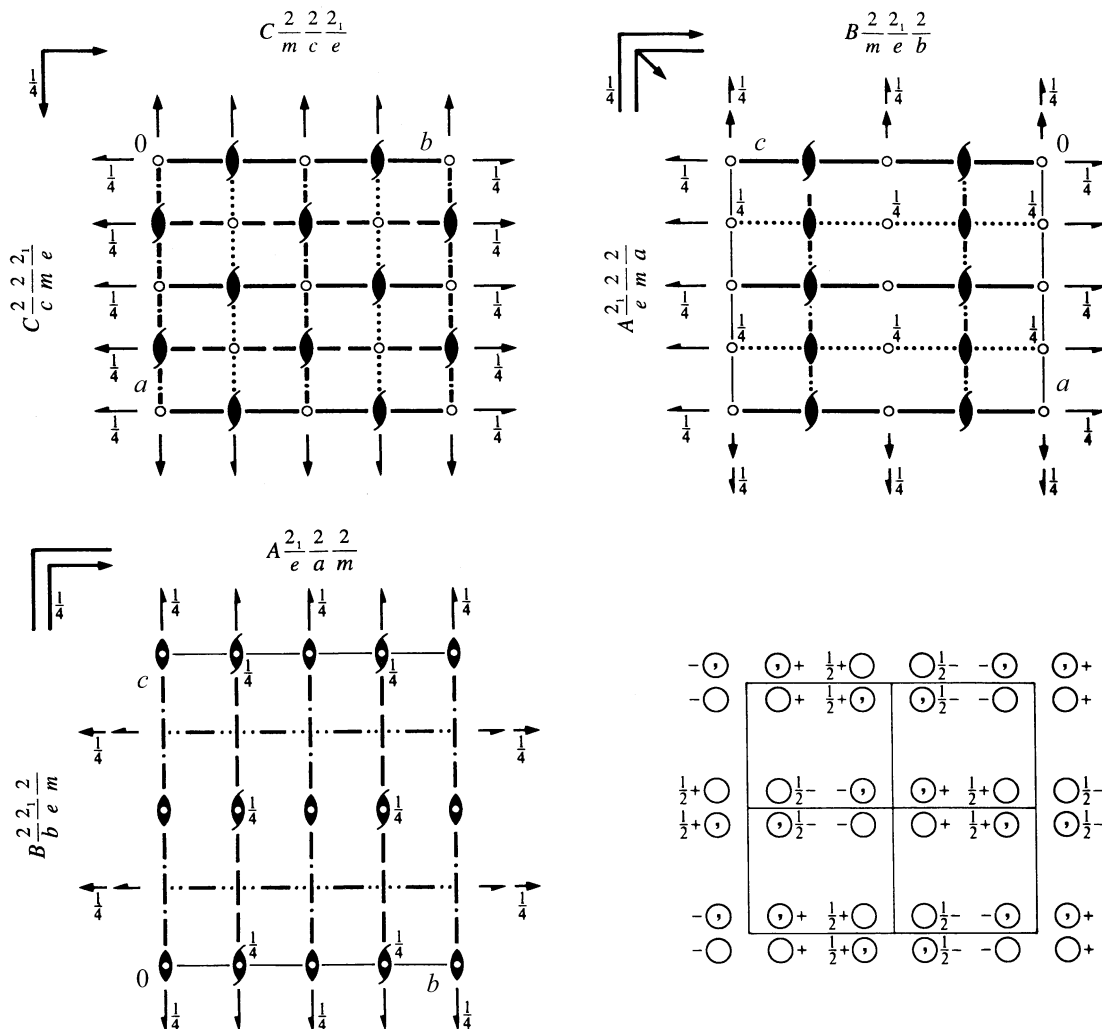
Orthorhombic

No. 64

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

Patterson symmetry *Cmmm*

Former space-group symbol *Cmca*; cf. Section 2.1.2



Origin at centre ($2/m$) at $2/mn1$

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

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

- (1) $t(\frac{1}{2}, \frac{1}{2}, 0)$
- (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}, 0, z$
- (3) 2 $\frac{1}{4}, y, \frac{1}{4}$
- (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$
- (5) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$
- (6) a $x, y, \frac{1}{4}$
- (7) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$
- (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
16	<i>g</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) x,\bar{y},\bar{z} (8) \bar{x},y,z	General: $hkl: h+k=2n$ $0kl: k=2n$ $h0l: h,l=2n$ $hk0: h,k=2n$ $h00: h=2n$ $0k0: k=2n$ $00l: l=2n$ Special: as above, plus no extra conditions
8	<i>f</i> $m..$	$0,y,z$	$0,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	<i>e</i> $.2.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{4}$	$hkl: h=2n$
8	<i>d</i> $2..$	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$	$x,\frac{1}{2},\frac{1}{2}$	$hkl: k+l=2n$
8	<i>c</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$hkl: k,l=2n$
4	<i>b</i> $2/m..$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl: k+l=2n$
4	<i>a</i> $2/m..$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl: k+l=2n$

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 $[100]$ $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along $[010]$ $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at $0,y,0$