

$Cmme$

D_{2h}^{21}

mmm

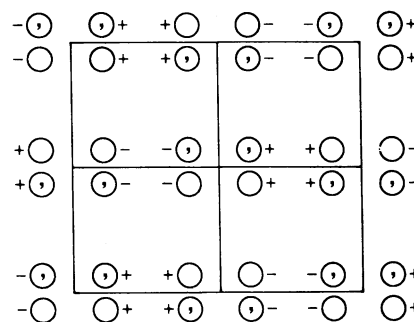
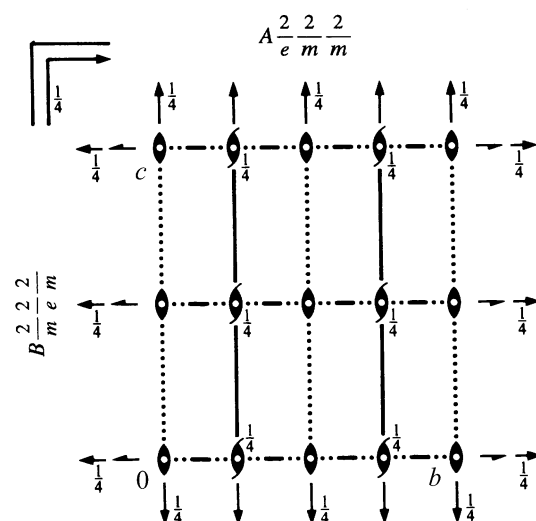
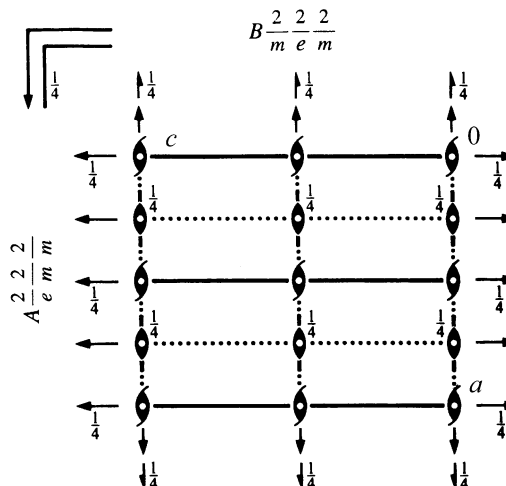
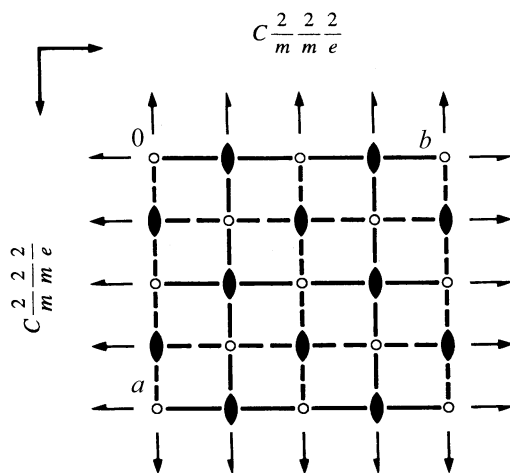
Orthorhombic

No. 67

$C 2/m 2/m 2/e$

Patterson symmetry $Cmmm$

Former space-group symbol $Cmma$; cf. Section 2.1.2



Origin at centre ($2/m$) at $2/m2_1/ae$

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

Symmetry operations

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

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

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

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

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

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] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

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