

Pcca

D_{2h}^8

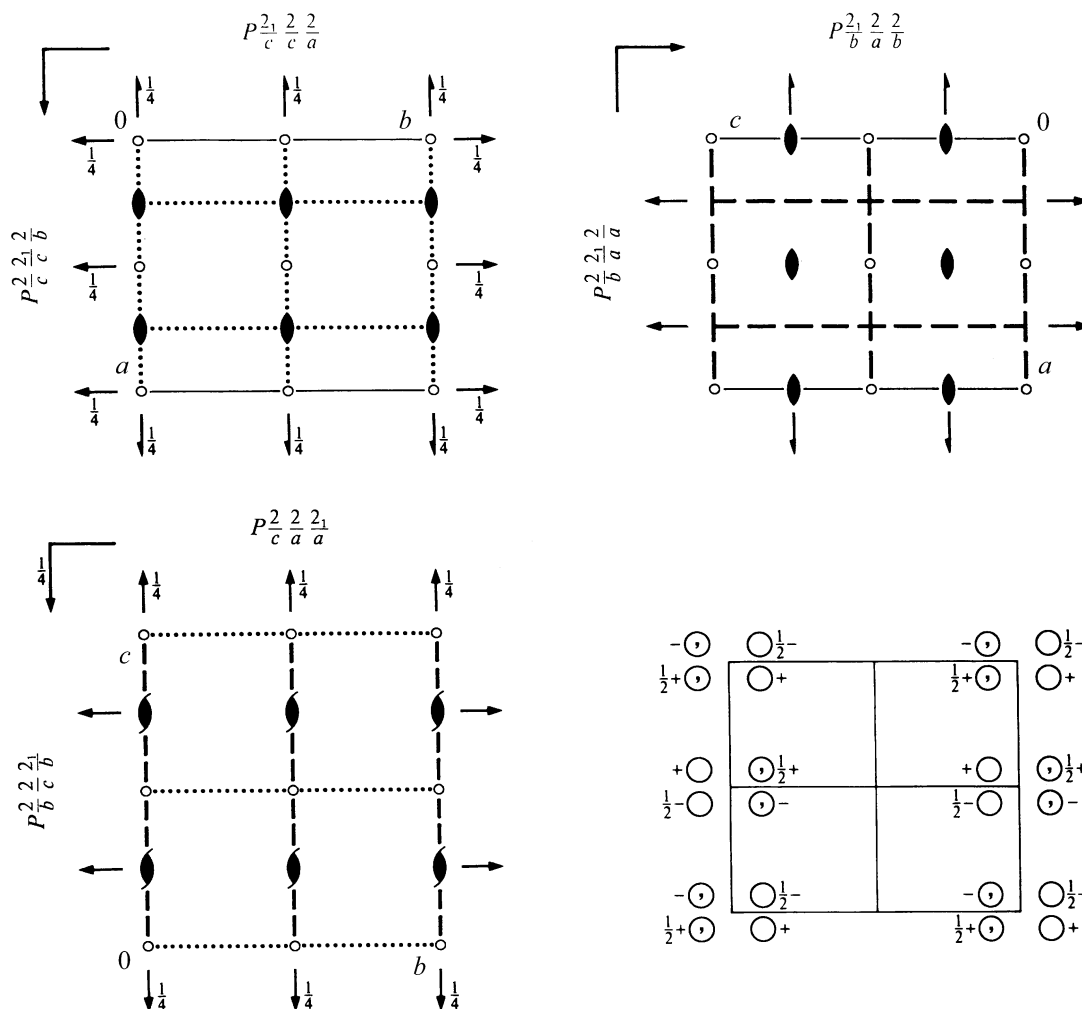
mmm

Orthorhombic

No. 54

$P 2_1/c 2/c 2/a$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1ca$

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

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

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

General:

$0kl: l = 2n$

$h0l: l = 2n$

$hk0: h = 2n$

$h00: h = 2n$

$00l: l = 2n$

Special: as above, plus

$hkl: l = 2n$

$hkl: l = 2n$

$hkl: h + l = 2n$

$hkl: h, l = 2n$

$hkl: h, l = 2n$

Symmetry of special projectionsAlong [001] $p2mm$

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

Origin at $0, 0, z$ Along [100] $p2mm$

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

Origin at $x, 0, 0$ Along [010] $p2gm$

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

Origin at $0, y, 0$