

Pccn

D_{2h}^{10}

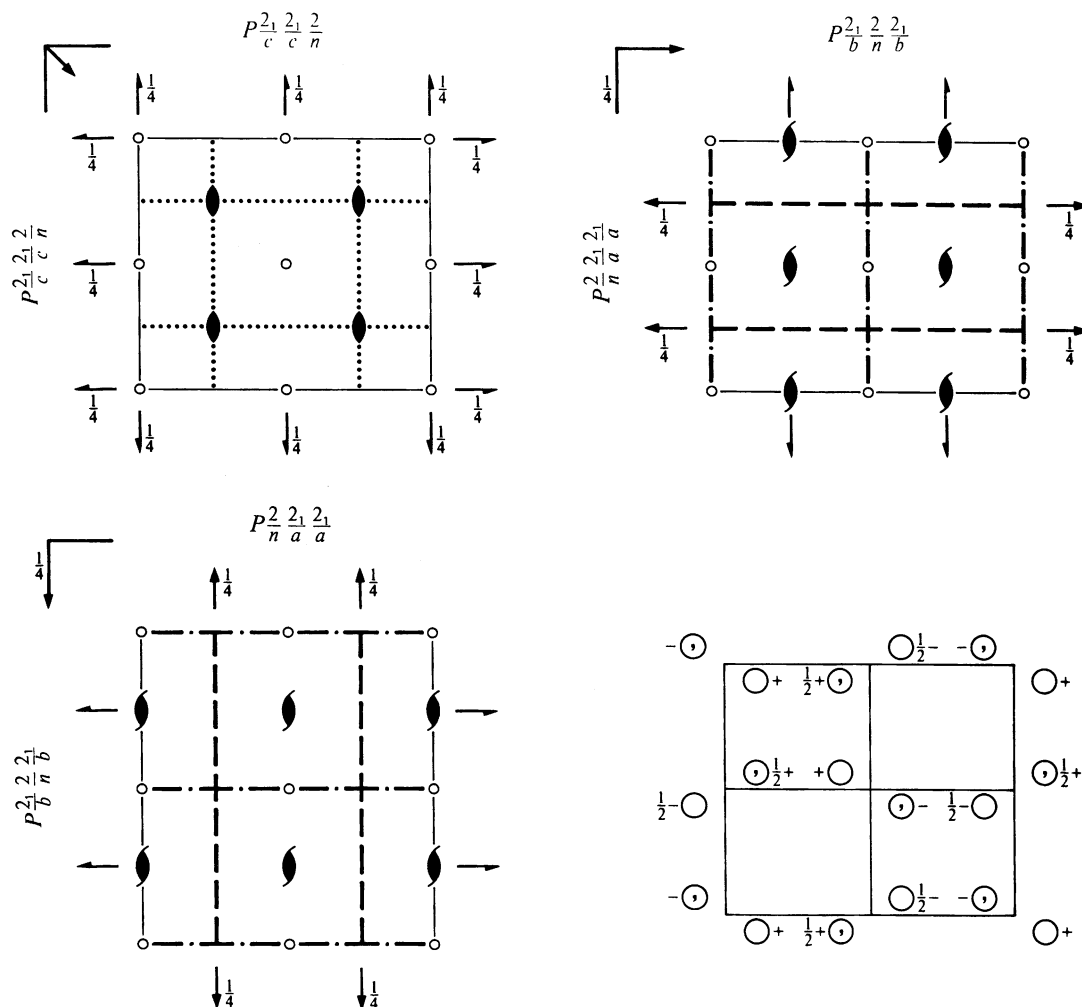
mmm

Orthorhombic

No. 56

$P 2_1/c 2_1/c 2/n$

Patterson symmetry *Pmmm*



Origin at $\bar{1}$ on $11n$

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

Symmetry operations

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

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
8 <i>e</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$	General: $0kl : l = 2n$ $h0l : l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>d</i> .. 2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>c</i> .. 2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pc2_1n$ ($Pna2_1, 33$)	1; 3; 6; 8
	[2] $P2_1cn$ ($Pna2_1, 33$)	1; 4; 6; 7
	[2] $Pcc2$ (27)	1; 2; 7; 8
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/c1$ ($P2_1/c, 14$)	1; 3; 5; 7
	[2] $P2_1/c11$ ($P2_1/c, 14$)	1; 4; 5; 8
	[2] $P112/n$ ($P2/c, 13$)	1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pccn$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (56); [3] $Pccn$ ($\mathbf{c}' = 3\mathbf{c}$) (56)

Minimal non-isomorphic supergroups

I [2] $P4/ncc$ (130); [2] $P4_2/ncm$ (138)

II [2] $Aema$ ($Cmce, 64$); [2] $Bmeb$ ($Cmce, 64$); [2] $Cccm$ (66); [2] $Ibam$ (72); [2] $Pccb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pcca, 54$); [2] $Pcca$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (54); [2] $Pmmn$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (59)