

$Pn\bar{1}m$

D_{2h}^{12}

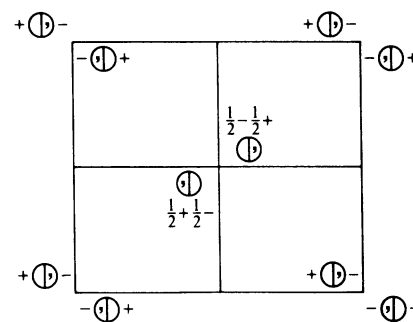
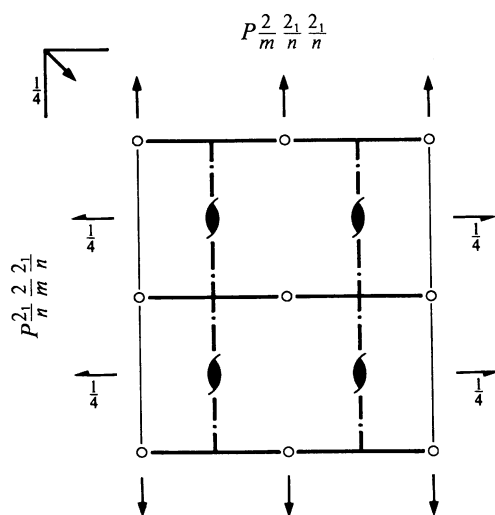
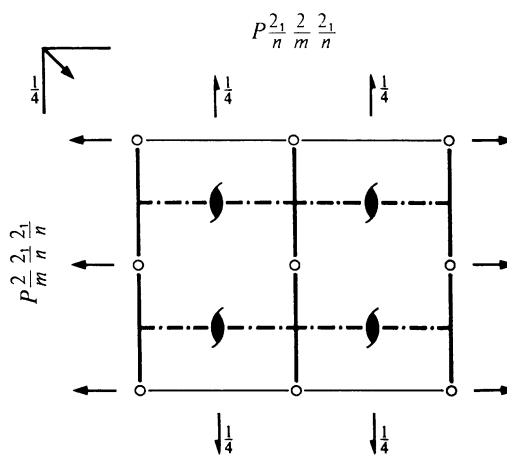
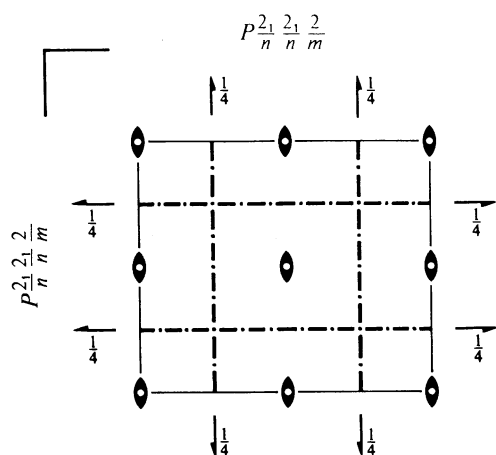
mmm

Orthorhombic

No. 58

$P 2_1/n 2_1/n 2/m$

Patterson symmetry $Pmmm$



Origin at centre ($2/m$)

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

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

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2_1m$ ($Pmn2_1$, 31)	1; 3; 6; 8
	[2] $P2_1nm$ ($Pmn2_1$, 31)	1; 4; 6; 7
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/n1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2_1/n11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnmm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (58); [3] $Pnmm$ ($\mathbf{c}' = 3\mathbf{c}$) (58)

Minimal non-isomorphic supergroups

I [2] $P4/mnc$ (128); [2] $P4_2/mnm$ (136)

II [2] $Amam$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Cccm$ (66); [2] $Immm$ (71); [2] $Pncm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmna$, 53); [2] $Pcnm$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmna$, 53); [2] $Pbam$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (55)