

Pnma

D_{2h}^{16}

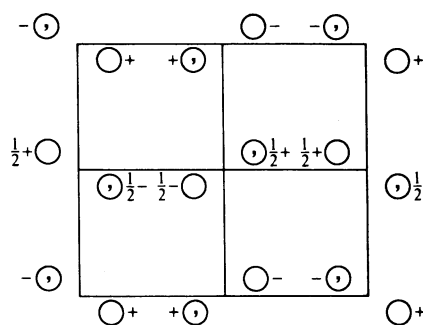
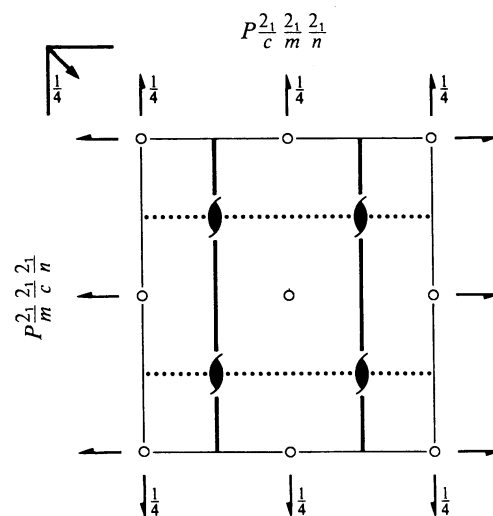
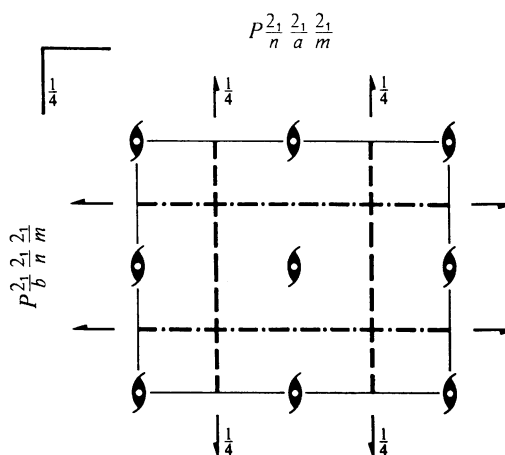
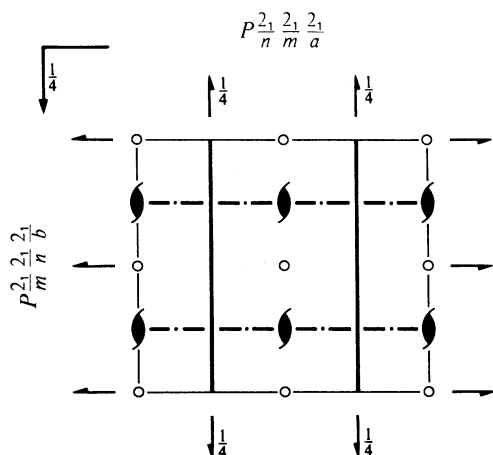
mmm

Orthorhombic

No. 62

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

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on 12, 1

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

Symmetry operations

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

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

Symmetry of special projections

Along [001] $p2gm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [010] $p2gg$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pn2_1a$ ($Pna2_1$, 33)	1; 3; 6; 8
	[2] $Pnm2_1$ ($Pmn2_1$, 31)	1; 2; 7; 8
	[2] $P2_1ma$ ($Pmc2_1$, 26)	1; 4; 6; 7
	[2] $P2_12_12_1$ (19)	1; 2; 3; 4
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/n11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12_1/m1$ ($P2_1/m$, 11)	1; 3; 5; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnma$ ($\mathbf{a}' = 3\mathbf{a}$) (62); [3] $Pnma$ ($\mathbf{b}' = 3\mathbf{b}$) (62); [3] $Pnma$ ($\mathbf{c}' = 3\mathbf{c}$) (62)

Minimal non-isomorphic supergroups

I none

II [2] $Amma$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Ccme$ ($Cmce$, 64); [2] $Imma$ (74); [2] $Pcma$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pbam$, 55); [2] $Pbma$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pbcm$, 57); [2] $Pnmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmnn$, 59)