

$Pn\bar{1}n$

D_{2h}^2

mmm

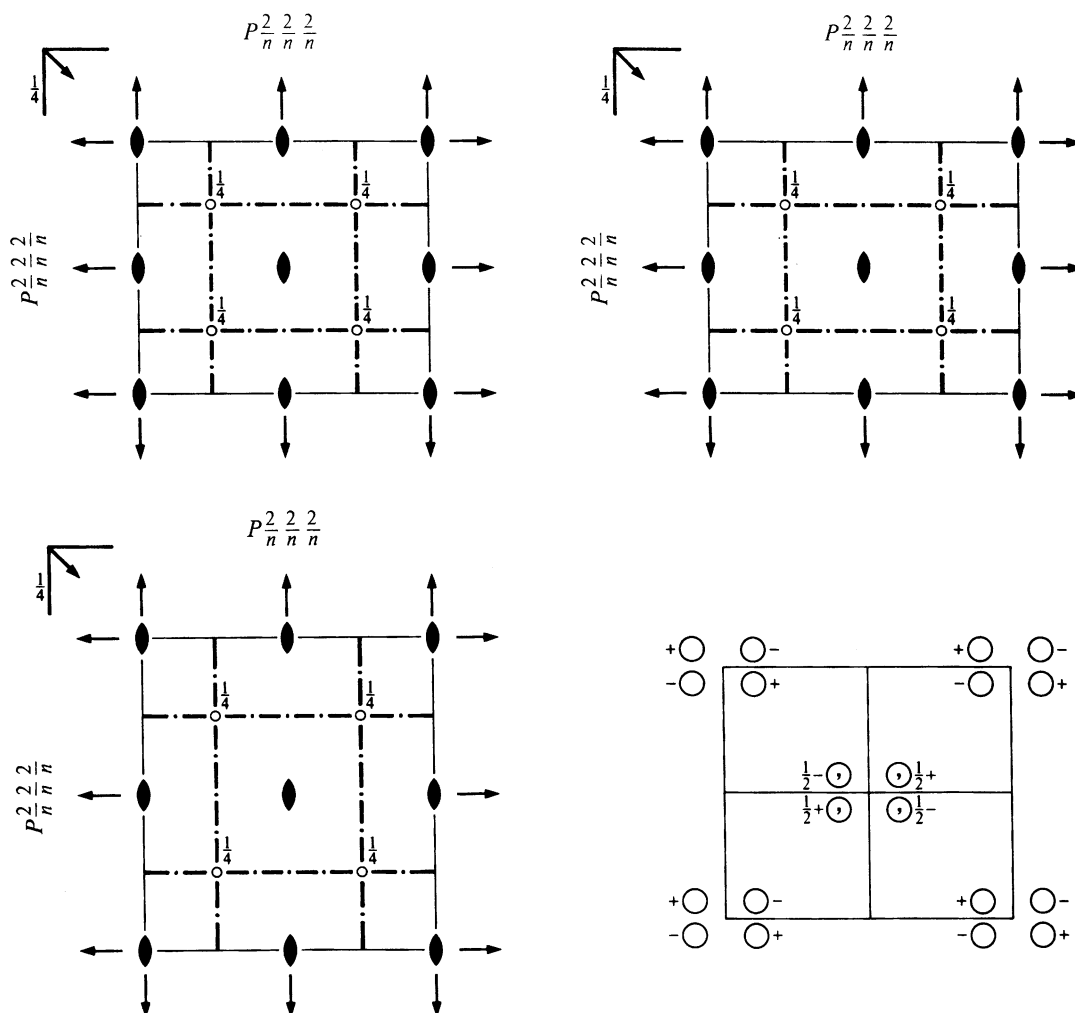
Orthorhombic

No. 48

$P 2/n 2/n 2/n$

Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at 222, at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{1}$

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

Symmetry operations

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

Minimal non-isomorphic supergroups

- I** [2] $P4/nnc$ (126); [2] $P4_2/nnm$ (134); [3] $Pn\bar{3}$ (201)
- II** [2] $Immm$ (71); [2] $Amaa(Cccm, 66)$; [2] $Bbmb(Cccm, 66)$; [2] $Cccm$ (66); [2] $Pncb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pban, 50$); [2] $Pcna$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pban, 50$); [2] $Pban$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (50)

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
						General:
8	<i>m</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) \bar{x}, y, \bar{z} (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) x, \bar{y}, \bar{z} (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	$Ok\bar{l} : k + l = 2n$ $h0\bar{l} : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00\bar{l} : l = 2n$
						Special: as above, plus
4	<i>l</i> ..2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>k</i> ..2	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>j</i> .2.	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, 0$	$0, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, y + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>i</i> .2.	$0, y, 0$	$0, \bar{y}, 0$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>h</i> 2..	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$x + \frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
4	<i>g</i> 2..	$x, 0, 0$	$\bar{x}, 0, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>f</i> $\bar{1}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4	<i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
2	<i>d</i> 222	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	<i>c</i> 222	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2	<i>b</i> 222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	<i>a</i> 222	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $c2mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

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] $Pn2n$ ($Pnn2$, 34)	1; 3; 6; 8
	[2] $P2nn$ ($Pnn2$, 34)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/n11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb [2] $Fddd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (70)

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnnn$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (48)

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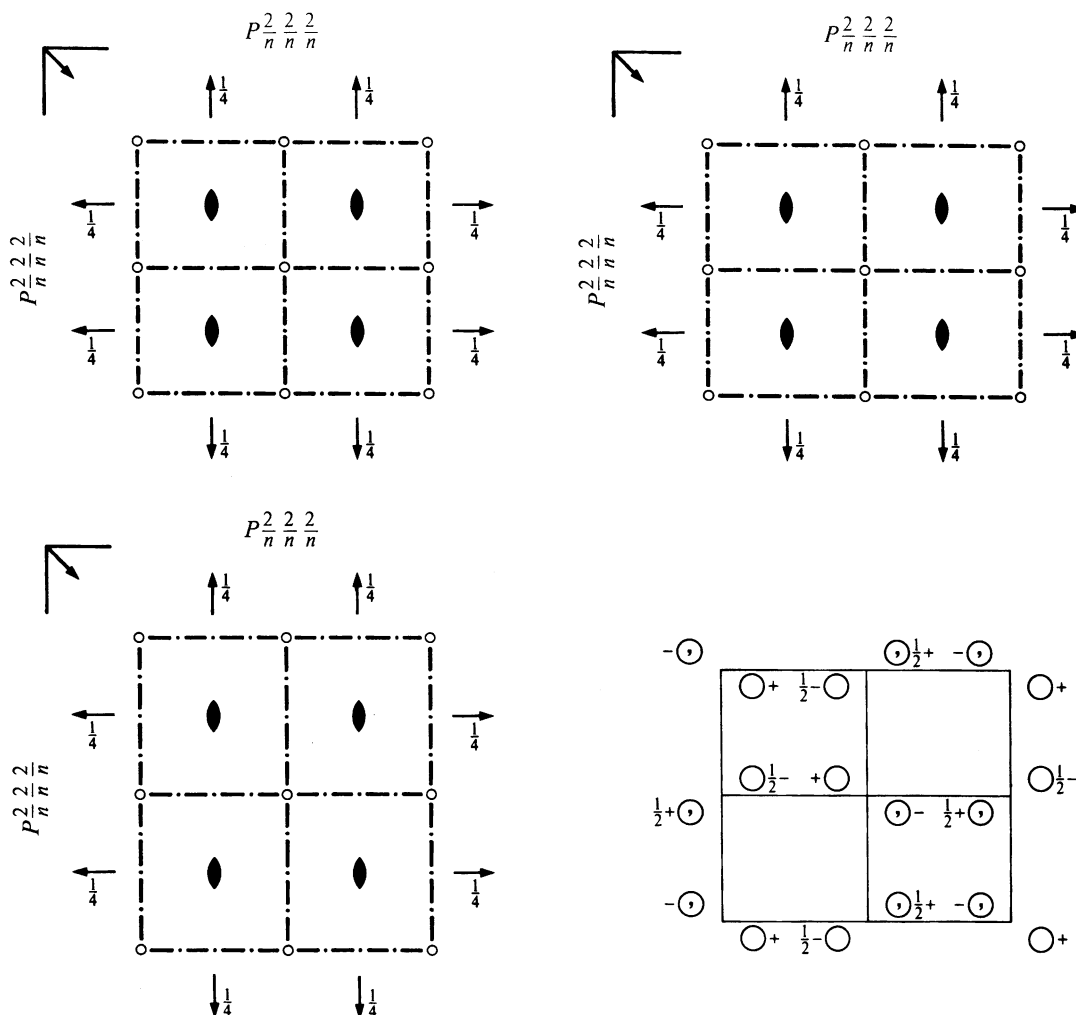
$Pn\bar{1}$ D_{2h}^2 mmm

Orthorhombic

No. 48

 $P 2/n 2/n 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at nnn , at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from 222Asymmetric unit $0 \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

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

Maximal isomorphic subgroups of lowest index

IIc [3] $Pn\bar{1}$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (48)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4_2/nm$ (134); [3] $Pn\bar{3}$ (201)II [2] $Immm$ (71); [2] $Amaa$ ($Cccm$, 66); [2] $Bbmb$ ($Cccm$, 66); [2] $Cccm$ (66); [2] $Pncb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pban$, 50); [2] $Pcna$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pban$, 50); [2] $Pban$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (50)

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
						General:
8	<i>m</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) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	$Ok\bar{l} : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$
						Special: as above, plus
4	<i>l</i> ..2	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>k</i> ..2	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	<i>j</i> .2.	$\frac{3}{4}, y, \frac{1}{4}$	$\frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4	<i>i</i> .2.	$\frac{1}{4}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, \bar{y}, \frac{3}{4}$	$\frac{3}{4}, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4	<i>h</i> 2..	$x, \frac{1}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
4	<i>g</i> 2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
4	<i>f</i> $\bar{1}$	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4	<i>e</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h + k, h + l, k + l = 2n$
2	<i>d</i> 222	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$
2	<i>c</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$			$hkl : h + k + l = 2n$
2	<i>b</i> 222	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$
2	<i>a</i> 222	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$			$hkl : h + k + l = 2n$

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] $c2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [010] $c2mm$

$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at $\frac{1}{4}, y, \frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
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