

$P4_2/n\,cm$

D_{4h}^{16}

$4/m\,mm$

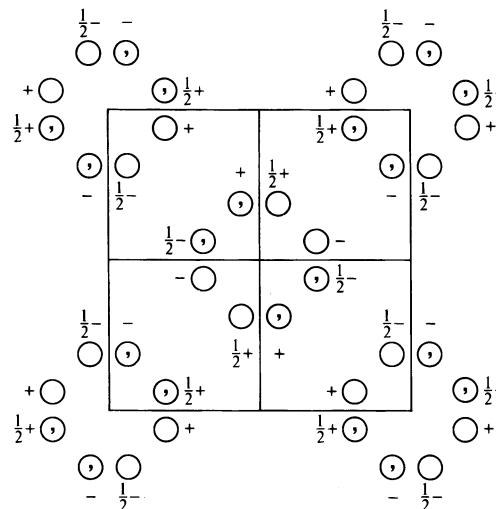
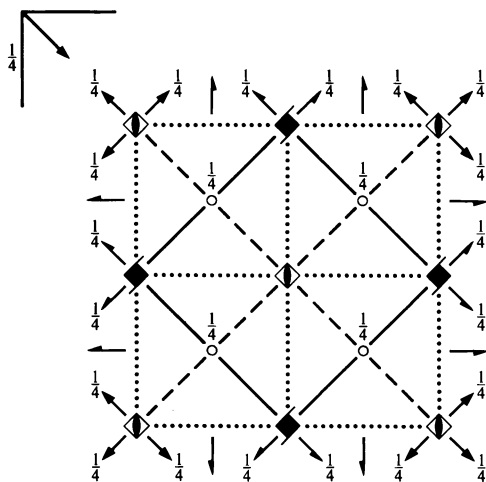
Tetragonal

No. 138

$P\ 4_2/n\ 2_1/c\ 2/m$

Patterson symmetry $P4/m\,mm$

ORIGIN CHOICE 1



Origin at $\bar{4}c$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from centre ($2/m$)

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

Symmetry operations

- | | | | |
|--|--|---|---|
| (1) 1 | (2) $2\ 0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})\ 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})\ \frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)\ \frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0)\ x, \frac{1}{4}, 0$ | (7) $2\ x, x, \frac{1}{4}$ | (8) $2\ x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}\ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)\ x, y, \frac{1}{4}$ | (11) $\bar{4}^+\ 0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-\ 0, 0, z; 0, 0, 0$ |
| (13) $c\ x, 0, z$ | (14) $c\ 0, y, z$ | (15) $m\ x + \frac{1}{2}, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0)\ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>j</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $0kl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$	
	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	
	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	
		Special: as above, plus
8 <i>i</i> .. <i>m</i>	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$	no extra conditions
	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$	
	$\bar{x}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	
	$x, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	
8 <i>h</i> .. 2	$x, x, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k = 2n$
	$\bar{x}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	
	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x, \bar{x}, \frac{1}{4}$	
	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x, \frac{1}{4}$	
8 <i>g</i> .. 2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k = 2n$
	$\bar{x}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$	
	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x, \bar{x}, \frac{3}{4}$	
	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	
8 <i>f</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $0, 0, \bar{z}$	
	$\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, z + \frac{1}{2}$	
	$0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z$	
4 <i>e</i> 2.. <i>mm</i>	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
	$\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	
4 <i>d</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	
4 <i>c</i> .. 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	
4 <i>b</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, 0$ $0, 0, \frac{1}{2}$	
4 <i>a</i> 2.. 22	$0, 0, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $0, 0, \frac{3}{4}$	

Symmetry of special projections

Along [001] $p4\,mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at 0, 0, z

Along [100] $p2\,mg$

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

Origin at $x, \frac{1}{4}, 0$

Along [110] $p2\,mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

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

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_2$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n\,cm$ ($\mathbf{c}' = 3\mathbf{c}$) (138); [9] $P4_2/n\,cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (138)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/m\,cm$ ($P4_2/m\,mc$, 131); [2] $I4/m\,cm$ (140); [2] $P4/n\,mm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)

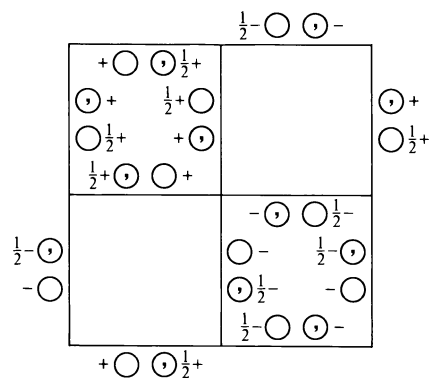
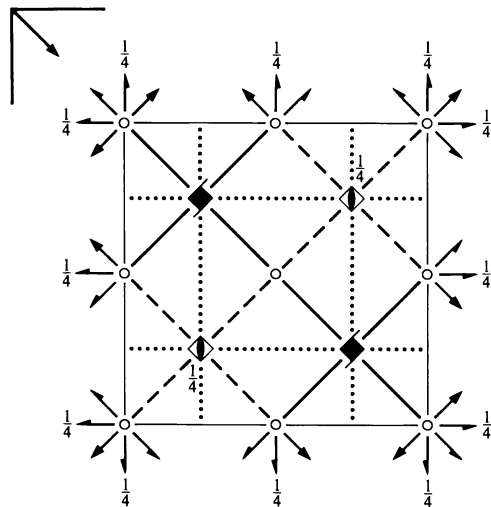
$P4_2/n\bar{c}m$ D_{4h}^{16} $4/m\bar{m}m$

Tetragonal

No. 138

 $P 4_2/n 2_1/c 2/m$ Patterson symmetry $P4/m\bar{m}m$

ORIGIN CHOICE 2

**Origin** at centre ($2/m$) at $n 1 (2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$ **Asymmetric unit** $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq y$ **Symmetry operations**

- | | | | |
|--|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) 0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (8) $2 x, \bar{x}, 0$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) $c x, \frac{1}{4}, z$ | (14) $c \frac{1}{4}, y, z$ | (15) $m x + \frac{1}{2}, \bar{x}, z$ | (16) $m x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>j</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (16) y, x, z	General: $hk0 : h + k = 2n$ $0kl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
8 <i>i</i> $\dots m$	x, x, z $\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, z + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $x, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8 <i>h</i> $\dots 2$	$x, \bar{x}, 0$ $\bar{x}, x, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>g</i> $\dots 2$	$x, \bar{x}, \frac{1}{2}$ $\bar{x}, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>f</i> $2\dots$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, z$	$hkl : h + k, l = 2n$
4 <i>e</i> $2\,mm$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	$hkl : l = 2n$
4 <i>d</i> $\dots 2/m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>c</i> $\dots 2/m$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>b</i> $\bar{4}\dots$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
4 <i>a</i> $2\,22$	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

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

Along $[100]$ $p2mg$

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

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
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IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n\,cm$ ($\mathbf{c}' = 3\mathbf{c}$) (138); [9] $P4_2/n\,cm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (138)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/m\,cm$ ($P4_2/m\,m\,c$, 131); [2] $I4/m\,c\,m$ (140); [2] $P4/n\,m\,m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)