

$P4/n$

C_{4h}^3

$4/m$

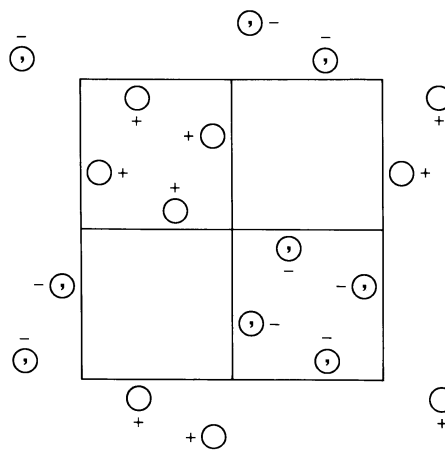
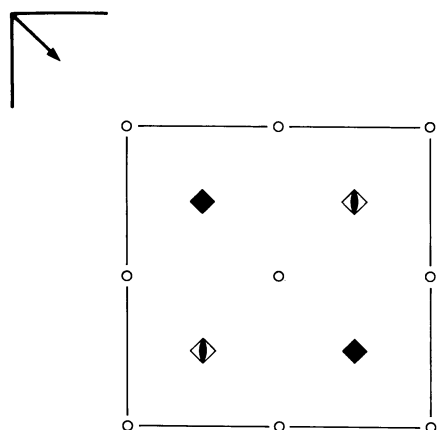
Tetragonal

No. 85

$P4/n$

Patterson symmetry $P4/m$

ORIGIN CHOICE 2



Origin at $\bar{1}$ on n , at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}$

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

Symmetry operations

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

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>g</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) $\bar{y} + \frac{1}{2}, x, z$ (7) $y + \frac{1}{2}, \bar{x}, \bar{z}$	(4) $y, \bar{x} + \frac{1}{2}, z$ (8) $\bar{y}, x + \frac{1}{2}, \bar{z}$	General: $hk0 : h + k = 2n$ $h00 : h = 2n$ Special: as above, plus $hkl : h + k = 2n$ $hkl : h, k = 2n$ $hkl : h, k = 2n$ no extra conditions $hkl : h + k = 2n$ $hkl : h + k = 2n$
4	<i>f</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$	$\frac{3}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, \bar{z}$	
4	<i>e</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	
4	<i>d</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	
2	<i>c</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$			
2	<i>b</i> $\bar{4}$..	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$			
2	<i>a</i> $\bar{4}$..	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$			

Symmetry of special projections

Along [001] $p4$

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

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

Along [100] $p2mg$

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

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] $P\bar{4}$ (81)	1; 2; 7; 8
	[2] $P4$ (75)	1; 2; 3; 4
	[2] $P2/n$ ($P2/c$, 13)	1; 2; 5; 6

IIa none

IIb [2] $P4_2/n$ ($c' = 2c$) (86)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/n$ ($c' = 2c$) (85); [5] $P4/n$ ($\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$) (85)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)