

*I*422

D_4^9

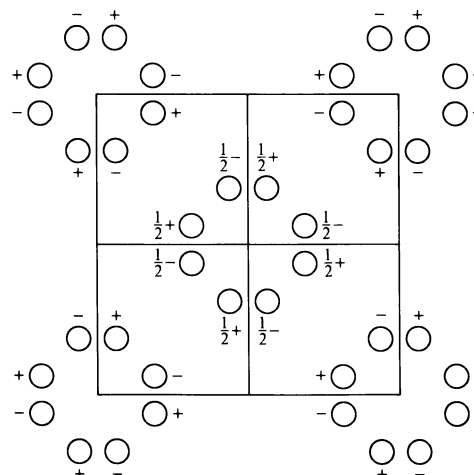
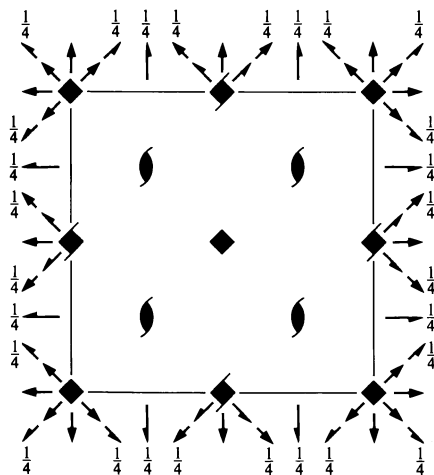
422

Tetragonal

No. 97

*I*422

Patterson symmetry *I*4/*m**m*



Origin at 422

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

Symmetry operations

For (0,0,0)+ set

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

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$	General:
16 <i>k</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{y}, x, z (4) y, \bar{x}, z (5) \bar{x}, y, \bar{z} (6) x, \bar{y}, \bar{z} (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8 <i>j</i> ..2	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	Special: as above, plus $0kl : k = 2n$
8 <i>i</i> .2.	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$	no extra conditions
8 <i>h</i> .2.	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$	no extra conditions
8 <i>g</i> ..2	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, x, 0$ $x, \bar{x}, 0$	no extra conditions
8 <i>f</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, \bar{z}$	$hkl : l = 2n$
4 <i>e</i> 4..	$0, 0, z$ $0, 0, \bar{z}$	no extra conditions
4 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$	$hkl : l = 2n$
4 <i>c</i> 222.	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : l = 2n$
2 <i>b</i> 422	$0, 0, \frac{1}{2}$	no extra conditions
2 <i>a</i> 422	$0, 0, 0$	no extra conditions

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 $0, 0, z$

Along [100] $c2mm$

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

Origin at $x, 0, 0$

Along [110] $p2mm$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $I411$ ($I4, 79$)	(1; 2; 3; 4)+
	[2] $I221$ ($I222, 23$)	(1; 2; 5; 6)+
	[2] $I212$ ($F222, 22$)	(1; 2; 7; 8)+
IIa	[2] $P4_2, 2$ (94)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2, 2$ (93)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2, 2$ (90)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
IIIb	none	

Maximal isomorphic subgroups of lowest index

IIIc [3] $I422$ ($\mathbf{c}' = 3\mathbf{c}$) (97); [9] $I422$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (97)

Minimal non-isomorphic supergroups

I	[2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $F432$ (209); [3] $I432$ (211)
II	[2] $C422$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P422, 89$)