

$I4$

C_4^5

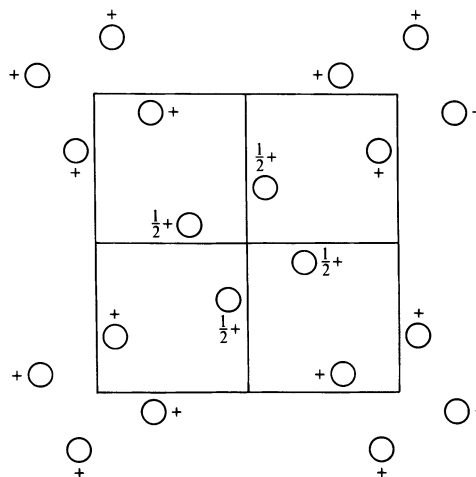
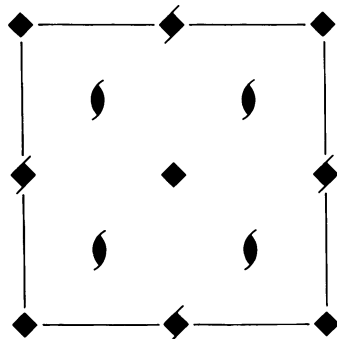
4

Tetragonal

No. 79

$I4$

Patterson symmetry $I4/m$



Origin on 4

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

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) 2 $0,0,z$ (3) $4^+ 0,0,z$ (4) $4^- 0,0,z$

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) $4^-(0,0,\frac{1}{2}) \frac{1}{2}, 0, z$

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)

Positions

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

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 $0, 0, z$

Along $[100] c1m1$

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

Origin at $x, 0, 0$

Along $[110] p1m1$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I $[2]I2(C2, 5) (1; 2) +$

IIa $[2]P4_2(77) 1; 2; (3; 4) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 $[2]P4(75) 1; 2; 3; 4$

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[3]I4(\mathbf{c}' = 3\mathbf{c})(79)$; $[5]I4(\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})(79)$

Minimal non-isomorphic supergroups

I $[2]I4/m(87)$; $[2]I422(97)$; $[2]I4mm(107)$; $[2]I4cm(108)$

II $[2]C4(\mathbf{c}' = \frac{1}{2}\mathbf{c})(P4, 75)$