

Tetragonal

4

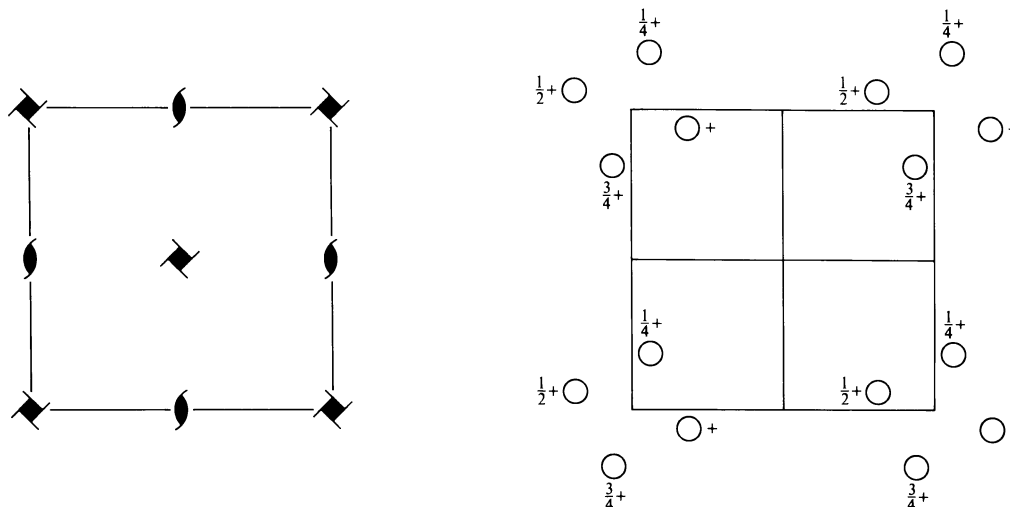
C_4^2

$P4_1$

Patterson symmetry $P4/m$

$P4_1$

No. 76



Origin on 4_1

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

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ 0,0,z (3) $4^+(0,0,\frac{1}{4})$ 0,0,z (4) $4^-(0,0,\frac{3}{4})$ 0,0,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
4 <i>a</i> 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{y},x,z+\frac{1}{4}$ (4) $y,\bar{x},z+\frac{3}{4}$	General: $00l : l = 4n$

Symmetry of special projections

Along $[001]$ $p4$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0,0,z

Along $[100]$ $p1g1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,0$

Along $[110]$ $p1g1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,x,0$

Maximal non-isomorphic subgroups

I $[2]P2_1(4)$ 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[2]C4_1(\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b})(P4_1, 76)$; $[3]P4_3(\mathbf{c}' = 3\mathbf{c})(78)$; $[5]P4_1(\mathbf{c}' = 5\mathbf{c})(76)$

Minimal non-isomorphic supergroups

I $[2]P4_122(91)$; $[2]P4_12_12(92)$

II $[2]I4_1(80)$; $[2]P4_2(\mathbf{c}' = \frac{1}{2}\mathbf{c})(77)$