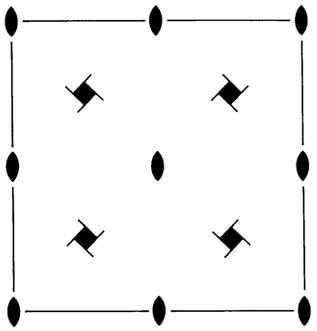
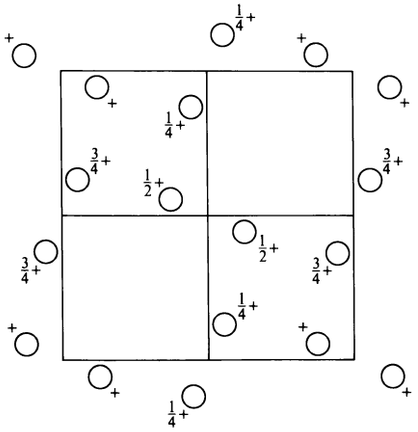
$I4_1$ C_4^6 4 Tetragonal

No. 80 $I4_1$ Patterson symmetry $I4/m$





Origin on 2

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

Symmetry operations

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

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

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

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

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 $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
8 b 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	General: hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$
4 a 2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$			Special: as above, plus hkl : $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

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

IIa [2] $P4_3$ (78) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4_1$ (76) 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1$ ($\mathbf{c}'=3\mathbf{c}$) (80); [5] $I4_1$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (80)

Minimal non-isomorphic supergroups

I [2] $I4_1/a$ (88); [2] $I4_122$ (98); [2] $I4_1md$ (109); [2] $I4_1cd$ (110)

II [2] $C4_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2$, 77)