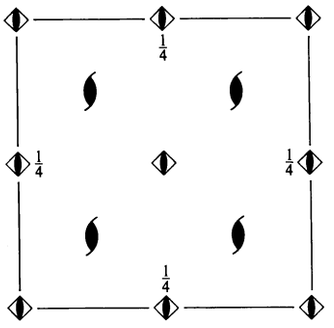
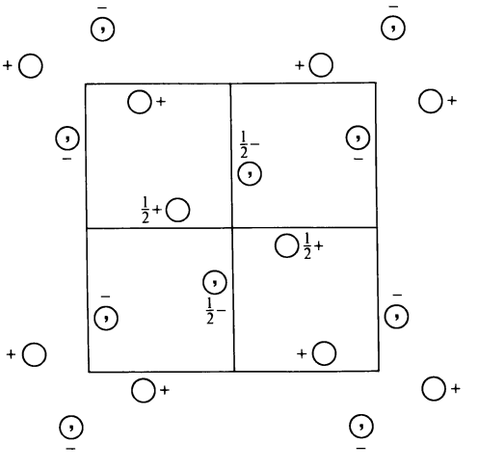
$I\bar{4}$ S_4^2 $\bar{4}$ Tetragonal

No. 82 $I\bar{4}$ Patterson symmetry $I4/m$





Origin at $\bar{4}$

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

Symmetry operations

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

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

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

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)

Positions

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

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 $0,0,z$

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] $P\bar{4}$ (81) 1; 2; 3; 4
[2] $P\bar{4}$ (81) $1;\ 2;\ (3;\ 4)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}$ ($\mathbf{c}' = 3\mathbf{c}$) (82); [5] $I\bar{4}$ ($\mathbf{a}' = \mathbf{a}+2\mathbf{b}, \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}-2\mathbf{b}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}$) (82)

Minimal non-isomorphic supergroups

I [2] $I4/m$ (87); [2] $I4_1/a$ (88); [2] $I\bar{4}m2$ (119); [2] $I\bar{4}c2$ (120); [2] $I\bar{4}2m$ (121); [2] $I\bar{4}2d$ (122)

II [2] $C\bar{4}$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P\bar{4}$, 81)