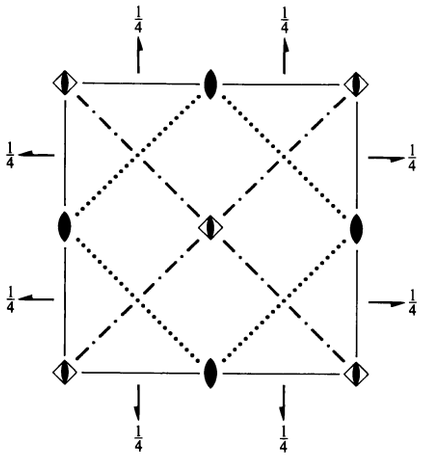
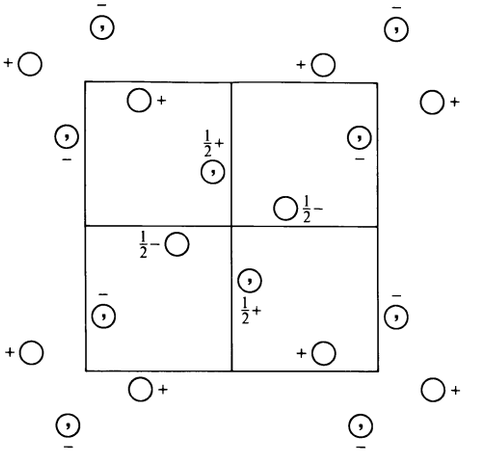
$P\bar{4}2_1c$ D_{2d}^4 $\bar{4}2m$ Tetragonal

No. 114 $P\bar{4}2_1c$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}1n$

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

(1) 1
(2) 2 $0,0,z$
(3) $\bar{4}^+$ $0,0,z$; $0,0,0$
(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(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) c $x+\frac{1}{2},\bar{x},z$
(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
							Special: as above, plus
4	*d*	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$ $hk0$: $h+k=2n$
4	*c*	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
2	*b*	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	*a*	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

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] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P22_11$ ($P2_12_12$, 18) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}2_1c$ ($\mathbf{c}'=3\mathbf{c}$) (114); [9] $P\bar{4}2_1c$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (114)

Minimal non-isomorphic supergroups

I [2] $P4/mnc$ (128); [2] $P4/ncc$ (130); [2] $P4_2/mbc$ (135); [2] $P4_2/nmc$ (137)

II [2] $C\bar{4}2c$ ($P\bar{4}c2$, 116); [2] $I\bar{4}2m$ (121); [2] $P\bar{4}2_1m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (113)