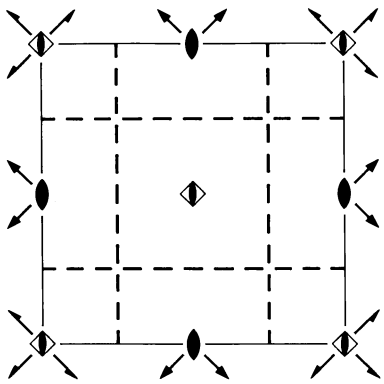
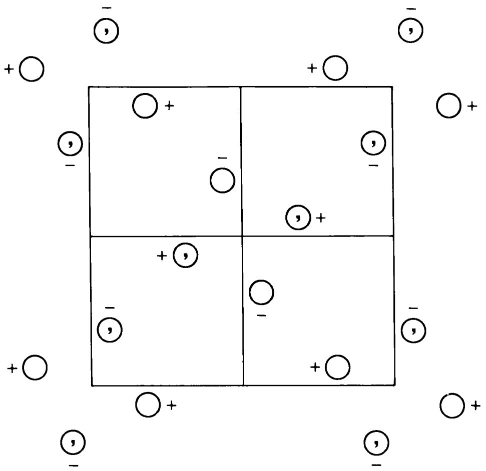
Tetragonal $\bar{4}m2$ D_{2d}^{7} $P\bar{4}b2$

Patterson symmetry $P4/mmm$ $P\bar{4}b2$ No. 117





Origin at $\bar{4}12_1$

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) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$

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	i	1	(1) x,y,z (5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $y,\bar{x},\bar{z}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	h	. . 2	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	no extra conditions
4	g	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$	no extra conditions
4	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	hkl: $h+k=2n$
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl: $h+k=2n$
2	d	2 . 22	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	c	2 . 22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

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

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

