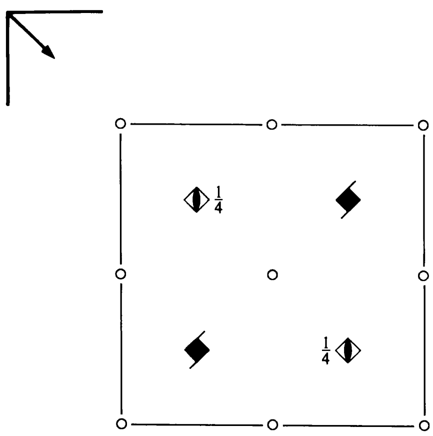
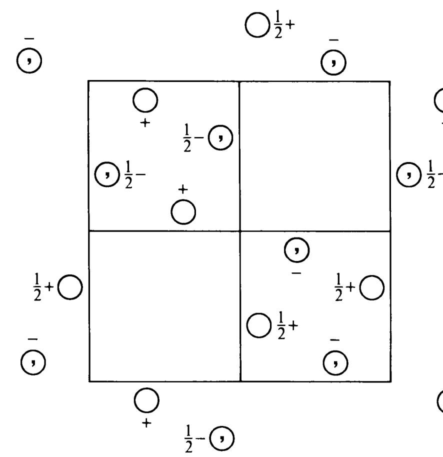
International Tables for Crystallography (2006). Vol. A, Space group 86, pp. 354–355.

$P4_2/n$ $\quad C_{4h}^4$ $\quad 4/m$ $\quad$ Tetragonal

No. 86 $\quad P4_2/n$ $\quad$ Patterson symmetry $P4/m$

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

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

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\ \ -\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{4},-\frac{1}{4},z$
(5) $\bar{1}\ \ 0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(7) $\bar{4}^+\ \ \frac{1}{4},\frac{1}{4},z;\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(8) $\bar{4}^-\ \ \frac{1}{4},\frac{1}{4},z;\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$

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	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
4	f	$2\,.\,.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
4	e	$2\,.\,.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl : $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
2	b	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl : $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k+l=2n$

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] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

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

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4_2$ (77) 1; 2; 3; 4
[2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $F4_1/d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/a$, 88)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n$ ($\mathbf{c}'=3\mathbf{c}$) (86); [5] $P4_2/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (86)

Minimal non-isomorphic supergroups

I [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II [2] $C4_2/m$ ($P4_2/m$, 84); [2] $I4/m$ (87); [2] $P4/n$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (85)