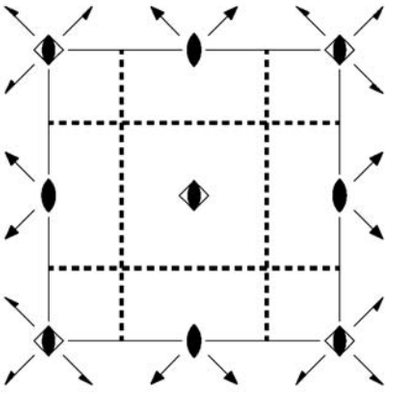
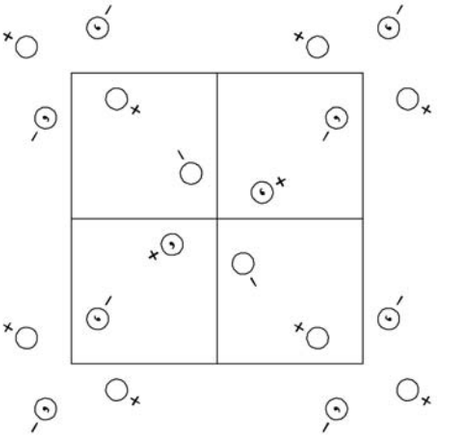
International Tables for Crystallography (2006). Vol. E, Layer group 60, pp. 344–345.

$p\bar{4}b2$ $\bar{4}m2$ Tetragonal/Square

No. 60 $p\bar{4}b2$ Patterson symmetry $p4/mmm$





Origin at $\bar{4}12_1$

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	$h0$: $h=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k$: $k=2n$
							Special: as above, plus
4	e	. . 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	d	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	hk: $h+k=2n$
4	c	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hk: $h+k=2n$
2	b	2 . 22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hk: $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hk: $h+k=2n$

Symmetry of special projections

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

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

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

Maximal non-isotypic subgroups

I [2] $p\bar{4}11$ ($p\bar{4}$, 50) 1; 2; 3; 4
[2] $p2b1$ ($pba2$, 25) 1; 2; 5; 6
[2] $p212$ ($c222$, 22) 1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p\bar{4}b2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (60)

Minimal non-isotypic supergroups

I [2] $p4/nbm$ (62); [2] $p4/mbm$ (63)

II [2] $c\bar{4}m2$ ($p\bar{4}2m$, 57)