

Tetragonal

$\bar{4}2m$

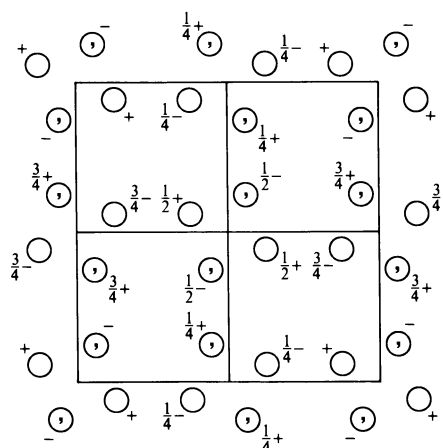
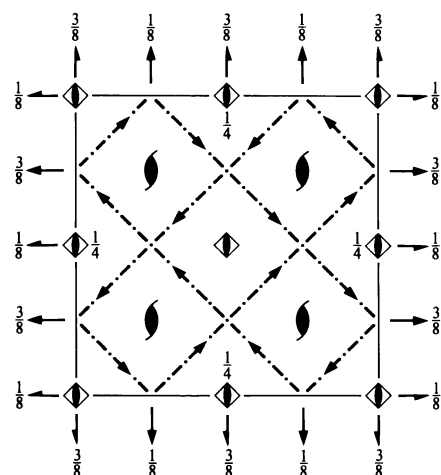
$D_{2d}^{12}$

$I\bar{4}2d$

Patterson symmetry  $I4/mmm$

$I\bar{4}2d$

No. 122



Origin at  $\bar{4}$

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

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

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

Generators selected (1);  $t(1,0,0); t(0,1,0); t(0,0,1); t(\frac{1}{2},\frac{1}{2},\frac{1}{2}); (2); (3); (5)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	General:
16 e 1	(1) $x,y,z$ (2) $\bar{x},\bar{y},z$ (3) $y,\bar{x},\bar{z}$ (4) $\bar{y},x,\bar{z}$ (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$ (6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{3}{4}$ (7) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $y+\frac{1}{2},x,z+\frac{3}{4}$	$hkl: h+k+l=2n$ $hk0: h+k=2n$ $0kl: k+l=2n$ $hhl: 2h+l=4n$ $00l: l=4n$ $h00: h=2n$ $h\bar{h}0: h=2n$
8 d .2.	$x,\frac{1}{4},\frac{1}{8}$ $\bar{x},\frac{3}{4},\frac{1}{8}$ $\frac{1}{4},\bar{x},\frac{7}{8}$ $\frac{3}{4},x,\frac{7}{8}$	Special: as above, plus no extra conditions
8 c 2..	$0,0,z$ $0,0,\bar{z}$ $\frac{1}{2},0,\bar{z}+\frac{3}{4}$ $\frac{1}{2},0,z+\frac{3}{4}$	$hkl: l=2n+1$ or $2h+l=4n$
4 b $\bar{4}$ ..	$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{4}$	$hkl: l=2n+1$ or $2h+l=4n$
4 a $\bar{4}$ ..	$0,0,0$ $\frac{1}{2},0,\frac{3}{4}$	$hkl: l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$ Origin at 0,0,z	Along [100] $c2mm$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x,0,\frac{3}{8}$	Along [110] $c1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x,x,0$
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