

Tetragonal

$4mm$

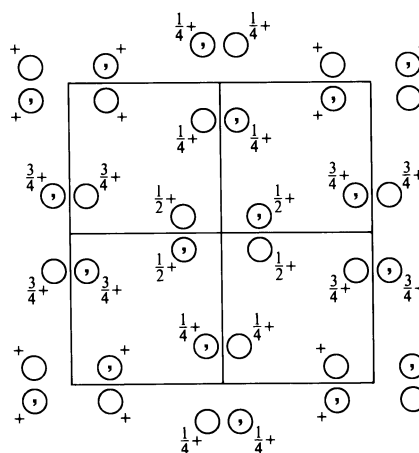
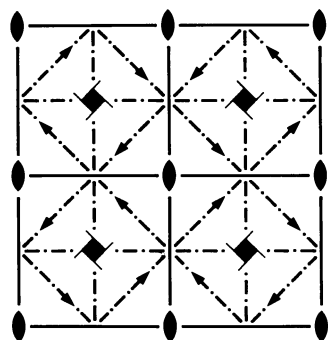
C_{4v}^{11}

$I4_1md$

Patterson symmetry $I4/mmm$

$I4_1md$

No. 109



Origin on $2mm$ on $2m1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

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

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

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

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	c	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	$hkl: h+k+l=2n$
			(5) x,\bar{y},z	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	(8) $y+\frac{1}{2},x,z+\frac{3}{4}$	$hk0: h+k=2n$

$0kl: k+l=2n$
 $hhl: 2h+l=4n$
 $00l: l=4n$
 $h00: h=2n$
 $h\bar{h}0: h=2n$

Special: as above, plus

no extra conditions

8	b	$.m.$	$0,y,z$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$	$y+\frac{1}{2},0,z+\frac{3}{4}$
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4	a	$2mm.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$			$hkl: l=2n+1$ or $2h+l=4n$
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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 $\frac{1}{4},\frac{1}{4},z$

Along $[100]$ $c1m1$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x,0,0$

Along $[110]$ $c1m1$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x,x,0$