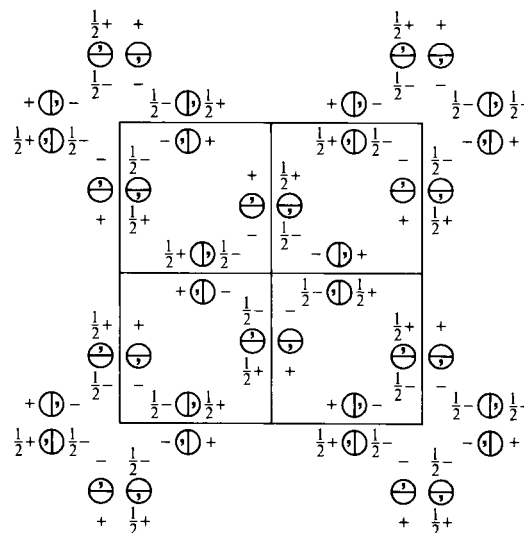
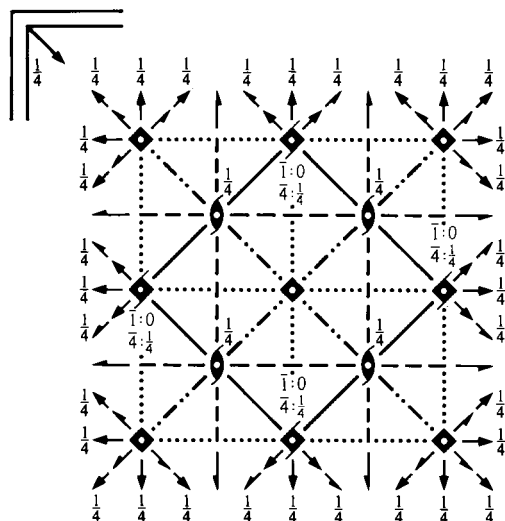


$I4/mcm$ D_{4h}^{18} $4/mmm$

Tetragonal

No. 140

 $I\ 4/m\ 2/c\ 2/m$ Patterson symmetry $I4/mmm$ Origin at centre ($4/m$) at $4/mc2_1/e$ Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; y \leq \frac{1}{2} - x$

Symmetry operations

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

- | | | | |
|--------------------------|--------------------------|-------------------------------|--------------------------------|
| (1) 1 | (2) $2\ 0,0,z$ | (3) $4^+ 0,0,z$ | (4) $4^- 0,0,z$ |
| (5) $2\ 0,y,\frac{1}{4}$ | (6) $2\ x,0,\frac{1}{4}$ | (7) $2\ x,x,\frac{1}{4}$ | (8) $2\ x,\bar{x},\frac{1}{4}$ |
| (9) $\bar{1}\ 0,0,0$ | (10) $m\ x,y,0$ | (11) $\bar{4}^+ 0,0,z; 0,0,0$ | (12) $\bar{4}^- 0,0,z; 0,0,0$ |
| (13) $c\ x,0,z$ | (14) $c\ 0,y,z$ | (15) $c\ x,\bar{x},z$ | (16) $c\ x,x,z$ |

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) $4^+(0,0,\frac{1}{2})\ 0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{2})\ \frac{1}{2},0,z$ |
| (5) $2(0,\frac{1}{2},0)\ \frac{1}{4},y,0$ | (6) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$ | (7) $2(\frac{1}{2},\frac{1}{2},0)\ x,x,0$ | (8) $2\ x,\bar{x}+\frac{1}{2},0$ |
| (9) $\bar{1}\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (10) $n(\frac{1}{2},\frac{1}{2},0)\ x,y,\frac{1}{4}$ | (11) $\bar{4}^+\ \frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$ | (12) $\bar{4}^- 0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$ |
| (13) $a\ x,\frac{1}{4},z$ | (14) $b\ \frac{1}{4},y,z$ | (15) $m\ x+\frac{1}{2},\bar{x},z$ | (16) $g(\frac{1}{2},\frac{1}{2},0)\ x,x,z$ |

Maximal non-isomorphic subgroups (continued)

- IIa**
- | | |
|----------------------|---|
| [2] $P4_2/ncm$ (138) | 1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4_2/mbc$ (135) | 1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4_2/nbc$ (133) | 1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4_2/mcm$ (132) | 1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4/ncc$ (130) | 1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4/mbm$ (127) | 1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4/nbm$ (125) | 1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ |
| [2] $P4/mcc$ (124) | 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16 |

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4/mcm$ ($c' = 3c$) (140); [9] $I4/mcm$ ($a' = 3a, b' = 3b$) (140)

Minimal non-isomorphic supergroups

I [3] $Fm\bar{3}c$ (226)**II** [2] $C4/mmm$ ($c' = \frac{1}{2}c$) ($P4/mmm$, 123)

Generators selected $(1); t(1,0,0); t(0,1,0); t(0,0,1); t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}); (2); (3); (5); (9)$

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				Reflection conditions
						General:
32	$m \quad 1$	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) x, y, \bar{z} (14) $\bar{x}, y, z + \frac{1}{2}$	(3) \bar{y}, x, z (7) $y, x, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) $y, x, z + \frac{1}{2}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k, l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$ Special: as above, plus
16	$l \quad \dots m$	$x, x + \frac{1}{2}, z$ $\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$	no extra conditions
16	$k \quad m \dots$	$x, y, 0$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, 0$ $y, x, \frac{1}{2}$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
16	$j \quad \dots 2$	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x}, 0, \frac{1}{4}$ $x, 0, \frac{3}{4}$	$0, x, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$	$0, \bar{x}, \frac{1}{4}$ $0, x, \frac{3}{4}$	$hkl : l=2n$
16	$i \quad \dots 2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x, x, \frac{3}{4}$	$\bar{x}, x, \frac{1}{4}$ $x, \bar{x}, \frac{3}{4}$	$x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$	$hkl : l=2n$
8	$h \quad m \dots 2m$	$x, x + \frac{1}{2}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x, 0$	$x + \frac{1}{2}, \bar{x}, 0$	no extra conditions
8	$g \quad 2 \dots mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : l=2n$
8	$f \quad 4 \dots$	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$	$hkl : l=2n$
8	$e \quad \dots 2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : k, l=2n$
4	$d \quad m \dots mm$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : l=2n$
4	$c \quad 4/m \dots$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l=2n$
4	$b \quad \bar{4} 2 m$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$			$hkl : l=2n$
4	$a \quad 4 2 2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l=2n$

Symmetry of special projections

Along $[001]$ $p4mm$

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

Origin at $0, 0, z$

Along $[100]$ $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	$[2] I\bar{4}2m (121)$	$(1; 2; 5; 6; 11; 12; 15; 16)+$
	$[2] I\bar{4}c2 (120)$	$(1; 2; 7; 8; 11; 12; 13; 14)+$
	$[2] I4cm (108)$	$(1; 2; 3; 4; 13; 14; 15; 16)+$
	$[2] I422 (97)$	$(1; 2; 3; 4; 5; 6; 7; 8)+$
	$[2] I4/m11 (I4/m, 87)$	$(1; 2; 3; 4; 9; 10; 11; 12)+$
	$[2] I2/m2/c1 (Ibam, 72)$	$(1; 2; 5; 6; 9; 10; 13; 14)+$
	$[2] I2/m12/m (Fmmm, 69)$	$(1; 2; 7; 8; 9; 10; 15; 16)+$

(Continued on preceding page)