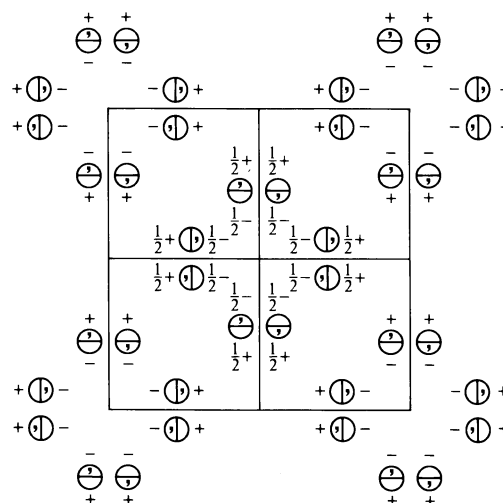
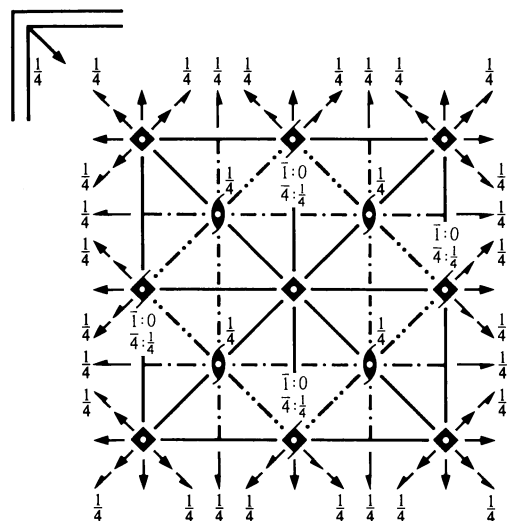


$I4/mmm$
 D_{4h}^{17}
 $4/mmm$

Tetragonal

No. 139

 $I 4/m 2/m 2/m$

 Patterson symmetry $I4/mmm$

Origin at centre ($4/mmm$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}; x \leq y$
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 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,0$ | (8) 2 $x,\bar{x},0$ |
| (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) m $x,0,z$ | (14) m $0,y,z$ | (15) m x,\bar{x},z | (16) m x,x,z |

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

- | | | | |
|---|---|---|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (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) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (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) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Maximal non-isomorphic subgroups (continued)

- IIa** [2] $P4_2/nmc$ (137) 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] $P4_2/mnm$ (136) 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] $P4_2/nnm$ (134) 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] $P4_2/mmc$ (131) 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] $P4/nmm$ (129) 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] $P4/nmc$ (128) 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] $P4/nnc$ (126) 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] $P4/mmm$ (123) 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] $I4/mmm$ ($c' = 3c$) (139); [9] $I4/mmm$ ($a' = 3a, b' = 3b$) (139)

Minimal non-isomorphic supergroups
I [3] $Fm\bar{3}m$ (225); [3] $Im\bar{3}m$ (229)

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

Symmetry of special projectionsAlong [001] $p4mm$

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

Origin at 0, 0, z

Along [100] $c2mm$

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

Origin at x, 0, 0

Along [110] $p2mm$

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

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] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+	
[2] $I4mm$ (107)	(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] $I2/m2/m1$ ($Immm$, 71)	(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)