

$I\bar{4}3m$

T_d^3

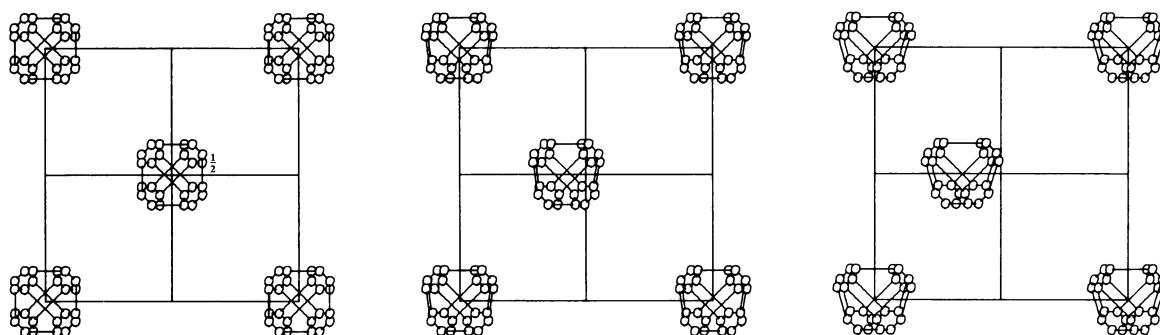
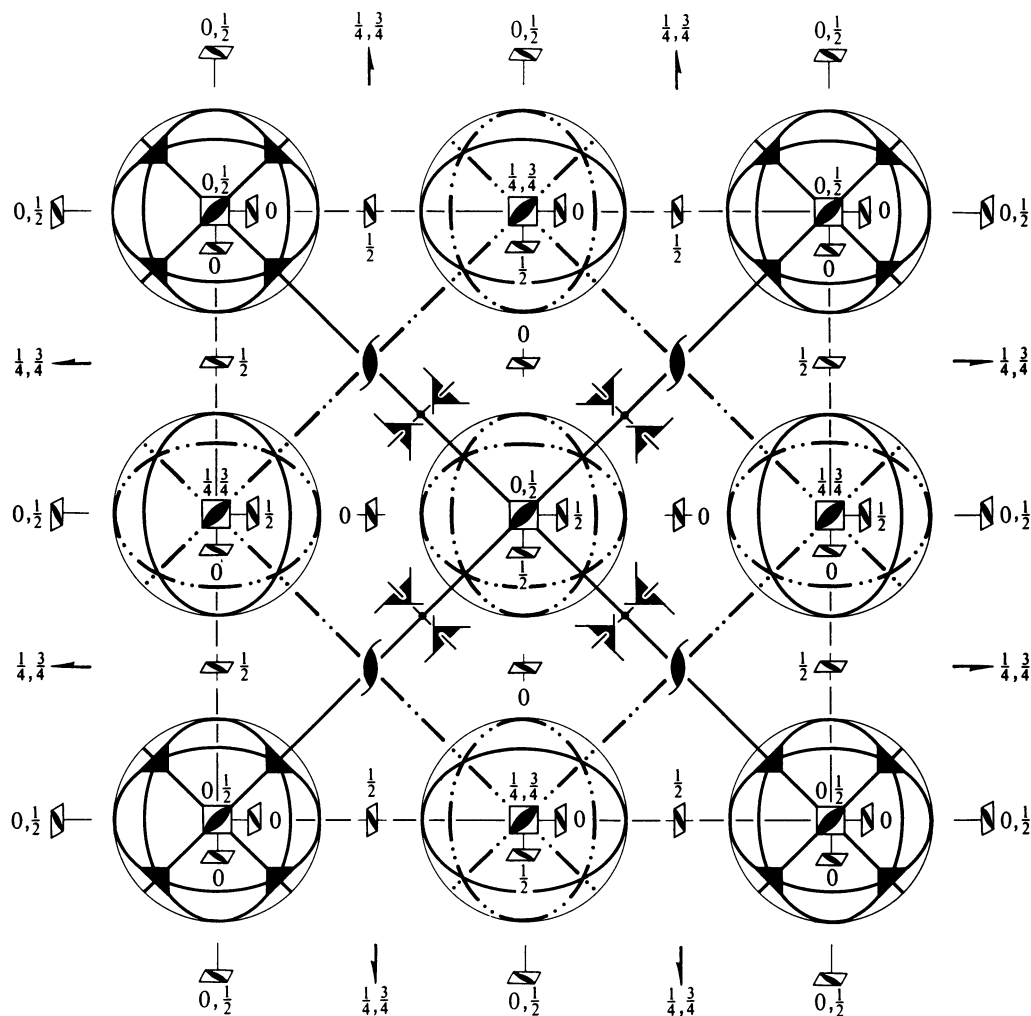
$\bar{4}3m$

Cubic

No. 217

$I\bar{4}3m$

Patterson symmetry $Im\bar{3}m$



Origin at $\bar{4}3m$

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

Symmetry operations

For (0,0,0)+ set

- | | | | |
|--------------------------|--|--|---|
| (1) 1 | (2) 2 0,0,z | (3) 2 0,y,0 | (4) 2 x,0,0 |
| (5) 3 ⁺ x,x,x | (6) 3 ⁺ \bar{x} ,x, \bar{x} | (7) 3 ⁺ x, \bar{x} , \bar{x} | (8) 3 ⁺ \bar{x} , \bar{x} ,x |
| (9) 3 ⁻ x,x,x | (10) 3 ⁻ x, \bar{x} , \bar{x} | (11) 3 ⁻ \bar{x} , \bar{x} ,x | (12) 3 ⁻ \bar{x} ,x, \bar{x} |
| (13) m x,x,z | (14) m x, \bar{x} ,z | (15) $\bar{4}^+$ 0,0,z; 0,0,0 | (16) $\bar{4}^-$ 0,0,z; 0,0,0 |
| (17) m x,y,y | (18) $\bar{4}^+$ x,0,0; 0,0,0 | (19) $\bar{4}^-$ x,0,0; 0,0,0 | (20) m x,y, \bar{y} |
| (21) m x,y,x | (22) $\bar{4}^-$ 0,y,0; 0,0,0 | (23) m \bar{x} ,y,x | (24) $\bar{4}^+$ 0,y,0; 0,0,0 |

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) 2(0, $\frac{1}{2}$,0) $\frac{1}{4}, y, \frac{1}{4}$ | (4) 2($\frac{1}{2}$,0,0) $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) 3 ⁺ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x | (6) 3 ⁺ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$ | (7) 3 ⁺ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$ | (8) 3 ⁺ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$ |
| (9) 3 ⁻ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x | (10) 3 ⁻ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$ | (11) 3 ⁻ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$ | (12) 3 ⁻ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$ |
| (13) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,x,z | (14) c $x + \frac{1}{2}, \bar{x}, z$ | (15) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (16) $\bar{4}^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (17) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,y,y | (18) $\bar{4}^+$ $x, \frac{1}{2}, 0; \frac{1}{4}, \frac{1}{2}, 0$ | (19) $\bar{4}^-$ $x, 0, \frac{1}{2}; \frac{1}{4}, 0, \frac{1}{2}$ | (20) a $x, y + \frac{1}{2}, \bar{y}$ |
| (21) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x,y,x | (22) $\bar{4}^-$ $\frac{1}{2}, y, 0; \frac{1}{2}, \frac{1}{4}, 0$ | (23) b $\bar{x} + \frac{1}{2}, y, x$ | (24) $\bar{4}^+$ $0, y, \frac{1}{2}; 0, \frac{1}{4}, \frac{1}{2}$ |

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); (13)

Positions

Multiplicity,	Coordinates	Reflection conditions
Wyckoff letter,	(0,0,0)+ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+	h, k, l permutable
Site symmetry		General:

- | | | | | | | | |
|----|---|---|------------|----------------------------|----------------------------|----------------------------|--|
| 48 | h | 1 | (1) x,y,z | (2) \bar{x}, \bar{y}, z | (3) \bar{x}, y, \bar{z} | (4) x, \bar{y}, \bar{z} | $hkl : h + k + l = 2n$
$0kl : k + l = 2n$
$hhl : l = 2n$
$h00 : h = 2n$ |
| | | | (5) z,x,y | (6) z, \bar{x}, \bar{y} | (7) \bar{z}, \bar{x}, y | (8) \bar{z}, x, \bar{y} | |
| | | | (9) y,z,x | (10) \bar{y}, z, \bar{x} | (11) y, \bar{z}, \bar{x} | (12) \bar{y}, \bar{z}, x | |
| | | | (13) y,x,z | (14) \bar{y}, \bar{x}, z | (15) y, \bar{x}, \bar{z} | (16) \bar{y}, x, \bar{z} | |
| | | | (17) x,z,y | (18) \bar{x}, z, \bar{y} | (19) \bar{x}, \bar{z}, y | (20) x, \bar{z}, \bar{y} | |
| | | | (21) z,y,x | (22) z, \bar{y}, \bar{x} | (23) \bar{z}, y, \bar{x} | (24) \bar{z}, \bar{y}, x | |

Special: no extra conditions

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|----|---|--------------|--|--|--|--|--|--|
| 24 | g | ..m | x,x,z
\bar{z}, \bar{x}, x | \bar{x}, \bar{x}, z
\bar{z}, x, \bar{x} | \bar{x}, x, \bar{z}
x,z,x | x, \bar{x}, \bar{z}
\bar{x}, z, \bar{x} | z,x,x
x, \bar{z}, \bar{x} | z, \bar{x}, \bar{x}
\bar{x}, \bar{z}, x |
| 24 | f | 2.. | $x, \frac{1}{2}, 0$
$\frac{1}{2}, x, 0$ | $\bar{x}, \frac{1}{2}, 0$
$\frac{1}{2}, \bar{x}, 0$ | $0, x, \frac{1}{2}$
$x, 0, \frac{1}{2}$ | $0, \bar{x}, \frac{1}{2}$
$\bar{x}, 0, \frac{1}{2}$ | $\frac{1}{2}, 0, x$
$0, \frac{1}{2}, x$ | $\frac{1}{2}, 0, \bar{x}$
$0, \frac{1}{2}, \bar{x}$ |
| 12 | e | 2.mm | x,0,0 | $\bar{x}, 0, 0$ | 0,x,0 | 0, $\bar{x}, 0$ | 0,0,x | 0,0, \bar{x} |
| 12 | d | $\bar{4}..$ | $\frac{1}{4}, \frac{1}{2}, 0$ | $\frac{3}{4}, \frac{1}{2}, 0$ | $0, \frac{1}{4}, \frac{1}{2}$ | $0, \frac{3}{4}, \frac{1}{2}$ | $\frac{1}{2}, 0, \frac{1}{4}$ | $\frac{1}{2}, 0, \frac{3}{4}$ |
| 8 | c | .3m | x,x,x | \bar{x}, \bar{x}, x | \bar{x}, x, \bar{x} | x, \bar{x}, \bar{x} | | |
| 6 | b | $\bar{4}2.m$ | $0, \frac{1}{2}, \frac{1}{2}$ | $\frac{1}{2}, 0, \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, 0$ | | | |
| 2 | a | $\bar{4}3m$ | 0,0,0 | | | | | |

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 [111] $p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x,x,x	Along [110] $p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at x,x,0
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Maximal non-isomorphic subgroups

- I** [2] $I231 (I23, 197)$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
 { [3] $I\bar{4}1m (I\bar{4}2m, 121)$ (1; 2; 3; 4; 13; 14; 15; 16)+
 [3] $I\bar{4}1m (I\bar{4}2m, 121)$ (1; 2; 3; 4; 17; 18; 19; 20)+
 [3] $I\bar{4}1m (I\bar{4}2m, 121)$ (1; 2; 3; 4; 21; 22; 23; 24)+
 { [4] $I13m (R3m, 160)$ (1; 5; 9; 13; 17; 21)+
 [4] $I13m (R3m, 160)$ (1; 6; 12; 14; 20; 21)+
 [4] $I13m (R3m, 160)$ (1; 7; 10; 14; 17; 23)+
 [4] $I13m (R3m, 160)$ (1; 8; 11; 13; 20; 23)+
- IIa** [2] $P\bar{4}3n (218)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
 [2] $P\bar{4}3m (215)$ 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
- IIb** none

Maximal isomorphic subgroups of lowest index

- IIc** [27] $I\bar{4}3m (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}) (217)$

Minimal non-isomorphic supergroups

- I** [2] $Im\bar{3}m (229)$
II [4] $P\bar{4}3m (\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}) (215)$