

$P4_2/nmc$

D_{4h}^{15}

$4/mmm$

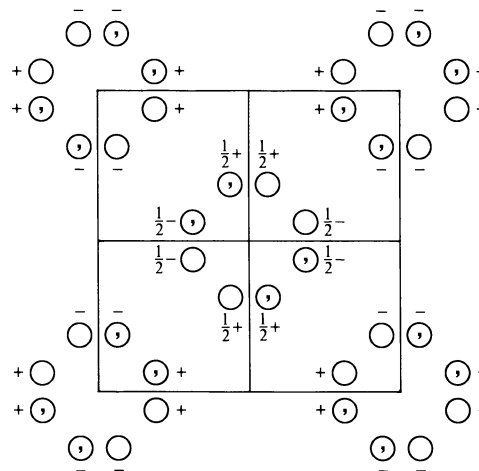
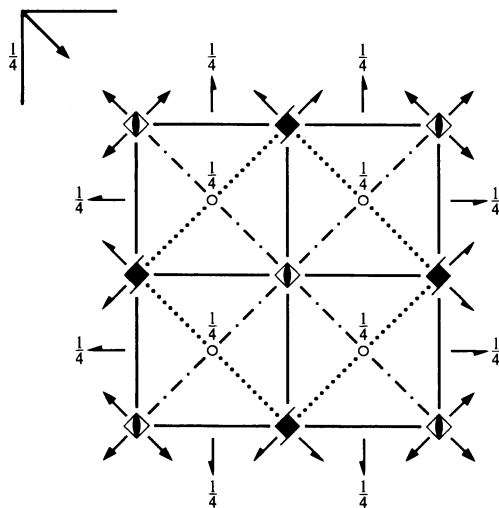
Tetragonal

No. 137

$P 4_2/n 2_1/m 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}m2/n$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

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

- | | | | |
|--|---|--|---|
| (1) 1 | (2) 2 $0, 0, z$ | (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 $x, x, 0$ | (8) 2 $x, \bar{x}, 0$ |
| (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) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) m $x, 0, z$ | (14) m $0, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

| Multiplicity, Wyckoff letter, Site symmetry | Coordinates | Reflection conditions |
|---|--|--|
| | | General: |
| 16 <i>h</i> 1 | (1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) x, \bar{y}, z | $hk0 : h + k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ |
| | (2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) \bar{x}, y, z | |
| | (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ | |
| | (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ | |
| | | Special: as above, plus |
| 8 <i>g</i> $.m.$ | $0, y, z$ $\frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ | $0, \bar{y}, z$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ |
| | $\bar{y} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $y, 0, \bar{z}$ | $y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\bar{y}, 0, \bar{z}$ |
| | | no extra conditions |
| 8 <i>f</i> $..2$ | $x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | $\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ |
| | $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x, \bar{x}, 0$ | $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, x, 0$ |
| | | $hkl : h + k + l = 2n$ |
| 8 <i>e</i> $\bar{1}$ | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ | $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ |
| | $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ | $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ |
| | | $hkl : h, k, l = 2n$ |
| 4 <i>d</i> $2mm.$ | $0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$ | $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ |
| | | $hkl : l = 2n$ |
| 4 <i>c</i> $2mm.$ | $0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ |
| | | $hkl : h + k + l = 2n$ |
| 2 <i>b</i> $\bar{4}m2$ | $0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ | |
| | | $hkl : h + k + l = 2n$ |
| 2 <i>a</i> $\bar{4}m2$ | $0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | |
| | | $hkl : h + k + l = 2n$ |

Symmetry of special projections

Along [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] $p2mg$

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

Origin at $x, \frac{1}{4}, \frac{1}{4}$

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] $P\bar{4}m2$ (115) | 1; 2; 7; 8; 11; 12; 13; 14 |
| | [2] $P\bar{4}_2c$ (114) | 1; 2; 5; 6; 11; 12; 15; 16 |
| | [2] $P4_2mc$ (105) | 1; 2; 3; 4; 13; 14; 15; 16 |
| | [2] $P4_22_2$ (94) | 1; 2; 3; 4; 5; 6; 7; 8 |
| | [2] $P4_2/n11$ ($P4_2/n$, 86) | 1; 2; 3; 4; 9; 10; 11; 12 |
| | [2] $P2/n12/c$ ($Ccce$, 68) | 1; 2; 7; 8; 9; 10; 15; 16 |
| | [2] $P2/n2_1/m1$ ($Pmnm$, 59) | 1; 2; 5; 6; 9; 10; 13; 14 |

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nmc$ ($\mathbf{c}' = 3\mathbf{c}$) (137); [9] $P4_2/nmc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (137)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/nmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)