

$R\bar{3}m$

D_{3d}^5

$\bar{3}m$

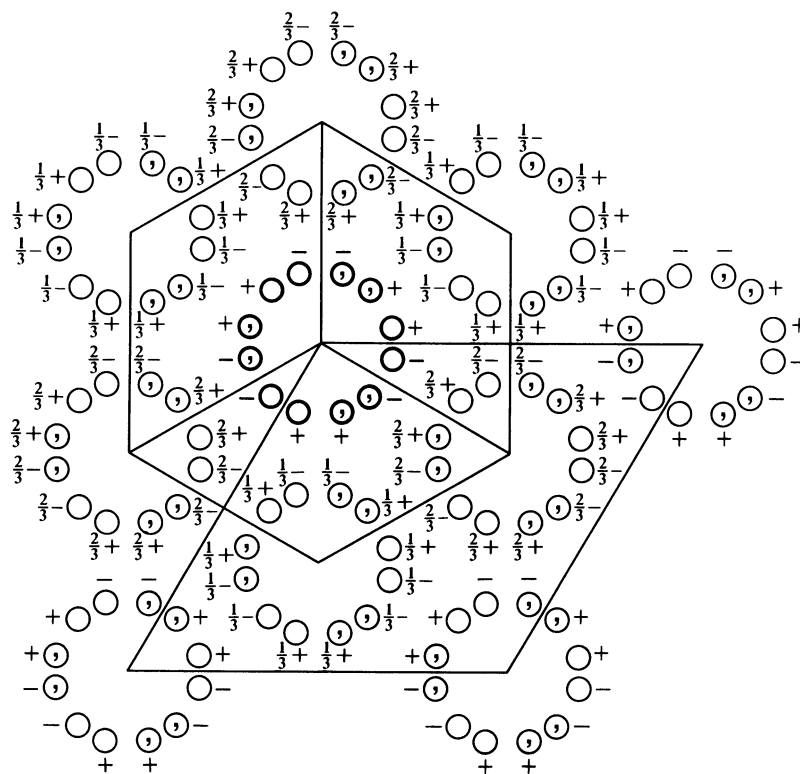
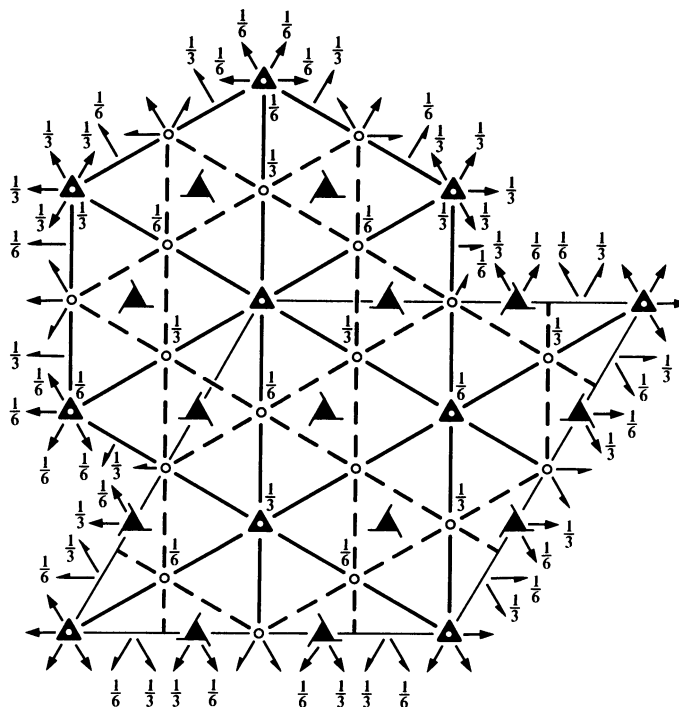
Trigonal

No. 166

$R\bar{3}2/m$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin at centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{6}$; $x \leq 2y$; $y \leq \min(1-x, 2x)$

Vertices $0, 0, 0$ $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
 $0, 0, \frac{1}{6}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{6}$ $\frac{1}{3}, \frac{2}{3}, \frac{1}{6}$

Symmetry operations

For (0,0,0)+ set

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

For $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ + set

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|--|--|--|
| (1) $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ | (2) $3^+(0,0,\frac{1}{3}) \frac{1}{3}, \frac{1}{3}, z$ | (3) $3^-(0,0,\frac{1}{3}) \frac{1}{3}, 0, z$ |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{6}, \frac{1}{6}$ | (5) $2(\frac{1}{2}, 0, 0) x, \frac{1}{6}, \frac{1}{6}$ | (6) $2 \frac{1}{3}, y, \frac{1}{6}$ |
| (7) $\bar{1} \frac{1}{3}, \frac{1}{6}, \frac{1}{6}$ | (8) $\bar{3}^+ \frac{1}{3}, -\frac{1}{3}, z; \frac{1}{3}, -\frac{1}{3}, \frac{1}{6}$ | (9) $\bar{3}^- \frac{1}{3}, \frac{2}{3}, z; \frac{1}{3}, \frac{2}{3}, \frac{1}{6}$ |
| (10) $g(\frac{1}{6}, -\frac{1}{6}, \frac{1}{3}) x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{6}, \frac{1}{3}, \frac{1}{3}) x + \frac{1}{4}, 2x, z$ | (12) $g(\frac{2}{3}, \frac{1}{3}, \frac{1}{3}) 2x, x, z$ |

For $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ + set

- | | | |
|--|--|--|
| (1) $t(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ | (2) $3^+(0,0,\frac{2}{3}) 0, \frac{1}{3}, z$ | (3) $3^-(0,0,\frac{2}{3}) \frac{1}{3}, \frac{1}{3}, z$ |
| (4) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{6}, \frac{1}{3}$ | (5) $2 x, \frac{1}{3}, \frac{1}{3}$ | (6) $2(0, \frac{1}{2}, 0) \frac{1}{6}, y, \frac{1}{3}$ |
| (7) $\bar{1} \frac{1}{6}, \frac{1}{3}, \frac{1}{3}$ | (8) $\bar{3}^+ \frac{2}{3}, \frac{1}{3}, z; \frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ | (9) $\bar{3}^- -\frac{1}{3}, \frac{1}{3}, z; -\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ |
| (10) $g(-\frac{1}{6}, \frac{1}{6}, \frac{2}{3}) x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{3}, \frac{2}{3}, \frac{2}{3}) x, 2x, z$ | (12) $g(\frac{1}{3}, \frac{1}{6}, \frac{2}{3}) 2x - \frac{1}{2}, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

(0,0,0)+ $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ +

- | | | | | | |
|----|----------|---|---------------------------------|-------------------------------|-------------------------------------|
| 36 | <i>i</i> | 1 | (1) x, y, z | (2) $\bar{y}, x - y, z$ | (3) $\bar{x} + y, \bar{x}, z$ |
| | | | (4) y, x, \bar{z} | (5) $x - y, \bar{y}, \bar{z}$ | (6) $\bar{x}, \bar{x} + y, \bar{z}$ |
| | | | (7) $\bar{x}, \bar{y}, \bar{z}$ | (8) $y, \bar{x} + y, \bar{z}$ | (9) $x - y, x, \bar{z}$ |
| | | | (10) \bar{y}, \bar{x}, z | (11) $\bar{x} + y, y, z$ | (12) $x, x - y, z$ |

Reflection conditions

General:

- $hkil : -h + k + l = 3n$
 $hki0 : -h + k = 3n$
 $hh\bar{2}hl : l = 3n$
 $h\bar{h}0l : h + l = 3n$
 $000l : l = 3n$
 $h\bar{h}00 : h = 3n$

Special: no extra conditions

- | | | | | | | | | |
|----|----------|------------|-------------------------------|-------------------------------|---|---------------------------|---------------------------|------------------------------|
| 18 | <i>h</i> | $.m$ | x, \bar{x}, z | $x, 2x, z$ | $2\bar{x}, \bar{x}, z$ | \bar{x}, x, \bar{z} | $2x, x, \bar{z}$ | $\bar{x}, 2\bar{x}, \bar{z}$ |
| 18 | <i>g</i> | $.2$ | $x, 0, \frac{1}{2}$ | $0, x, \frac{1}{2}$ | $\bar{x}, \bar{x}, \frac{1}{2}$ | $\bar{x}, 0, \frac{1}{2}$ | $0, \bar{x}, \frac{1}{2}$ | $x, x, \frac{1}{2}$ |
| 18 | <i>f</i> | $.2$ | $x, 0, 0$ | $0, x, 0$ | $\bar{x}, \bar{x}, 0$ | $\bar{x}, 0, 0$ | $0, \bar{x}, 0$ | $x, x, 0$ |
| 9 | <i>e</i> | $.2/m$ | $\frac{1}{2}, 0, 0$ | $0, \frac{1}{2}, 0$ | $\frac{1}{2}, \frac{1}{2}, 0$ | | | |
| 9 | <i>d</i> | $.2/m$ | $\frac{1}{2}, 0, \frac{1}{2}$ | $0, \frac{1}{2}, \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | | | |
| 6 | <i>c</i> | $3m$ | $0, 0, z$ | $0, 0, \bar{z}$ | | | | |
| 3 | <i>b</i> | $\bar{3}m$ | $0, 0, \frac{1}{2}$ | | | | | |
| 3 | <i>a</i> | $\bar{3}m$ | $0, 0, 0$ | | | | | |

Symmetry of special projections

Along [001] $p6mm$

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$
 Origin at 0, 0, z

Along [100] $p2$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$
 Origin at x, 0, 0

Along [210] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
 Origin at $x, \frac{1}{2}x, 0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

- I** [2] $R\bar{3}m$ (160) (1; 2; 3; 10; 11; 12)+
 [2] $R\bar{3}2$ (155) (1; 2; 3; 4; 5; 6)+
 [2] $R\bar{3}1$ ($R\bar{3}$, 148) (1; 2; 3; 7; 8; 9)+
 { [3] $R12/m$ ($C2/m$, 12) (1; 4; 7; 10)+
 [3] $R12/m$ ($C2/m$, 12) (1; 5; 7; 11)+
 [3] $R12/m$ ($C2/m$, 12) (1; 6; 7; 12)+
- IIa** { [3] $P\bar{3}m1$ (164) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
 [3] $P\bar{3}m1$ (164) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
 [3] $P\bar{3}m1$ (164) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
- IIb** [2] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (167)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (166)

Minimal non-isomorphic supergroups

- I** [4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)
- II** [3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (162)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

- I** [2] $R\bar{3}m$ (160) 1; 2; 3; 10; 11; 12
 [2] $R\bar{3}2$ (155) 1; 2; 3; 4; 5; 6
 [2] $R\bar{3}1$ ($R\bar{3}$, 148) 1; 2; 3; 7; 8; 9
 { [3] $R12/m$ ($C2/m$, 12) 1; 4; 7; 10
 [3] $R12/m$ ($C2/m$, 12) 1; 5; 7; 11
 [3] $R12/m$ ($C2/m$, 12) 1; 6; 7; 12
- IIa** none
- IIb** [2] $F\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($R\bar{3}c$, 167); [3] $P\bar{3}m1$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$) (164)

Maximal isomorphic subgroups of lowest index

- IIc** [2] $R\bar{3}m$ ($\mathbf{a}' = \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} - \mathbf{c}$) (166)

Minimal non-isomorphic supergroups

- I** [4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)
- II** [3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$) (162)