

$R\bar{3}2$

D_3^7

32

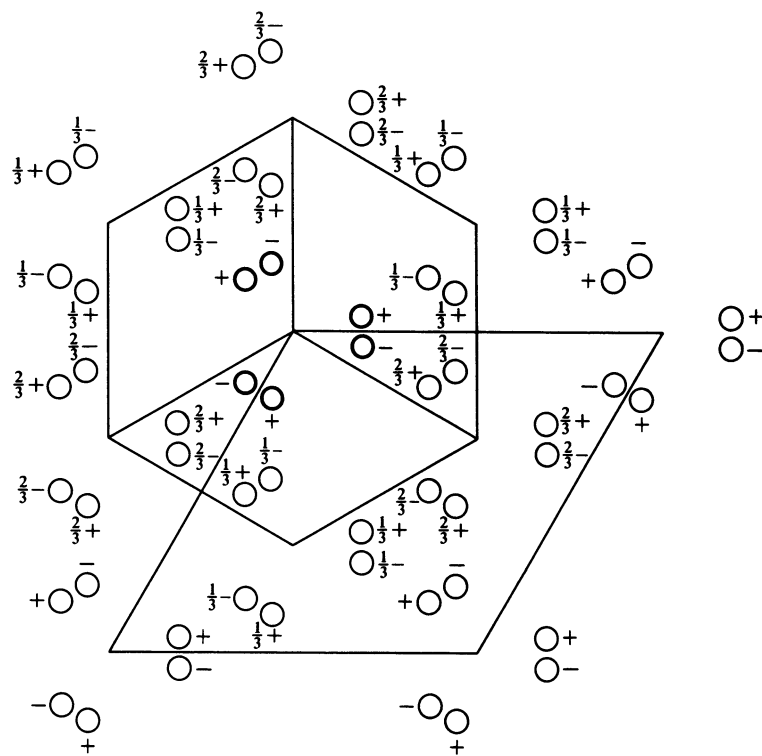
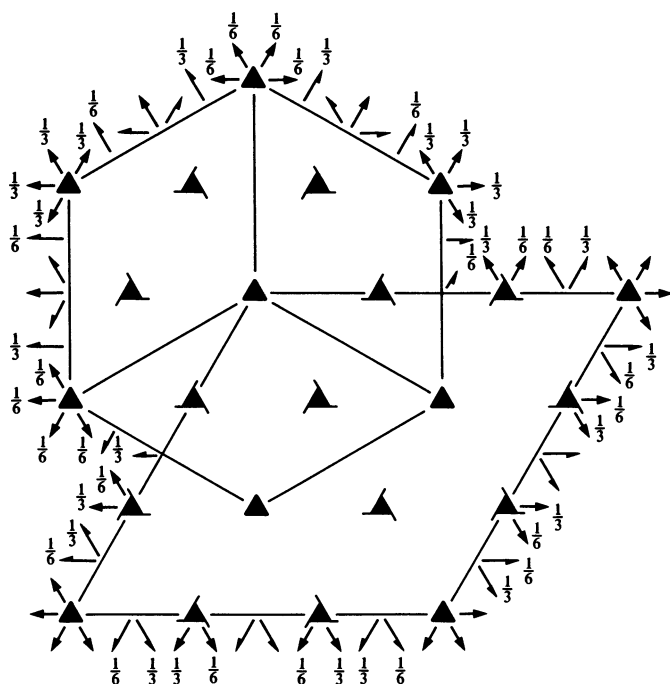
Trigonal

No. 155

$R\bar{3}2$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin at 32

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

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

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) $2 0,y,0$ |

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

- | | | |
|--|--|--|
| (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) $2 \frac{1}{3}, y, \frac{1}{6}$ |

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) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{6}, \frac{1}{6}$ | (5) $2 x, \frac{1}{3}, \frac{1}{3}$ | (6) $2(0, \frac{1}{2}, 0) \frac{1}{6}, y, \frac{1}{3}$ |

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)**Positions**

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

- | | | | | | |
|----|----------|---|-------------------|---------------------------|---------------------------------|
| 18 | <i>f</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) $\bar{x},\bar{x}+y,\bar{z}$ |

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

- | | | | | | |
|---|----------|----|-------------------|-------------------|-------------------------------|
| 9 | <i>e</i> | .2 | $x,0,\frac{1}{2}$ | $0,x,\frac{1}{2}$ | $\bar{x},\bar{x},\frac{1}{2}$ |
| 9 | <i>d</i> | .2 | $x,0,0$ | $0,x,0$ | $\bar{x},\bar{x},0$ |
| 6 | <i>c</i> | 3. | $0,0,z$ | $0,0,\bar{z}$ | |
| 3 | <i>b</i> | 32 | $0,0,\frac{1}{2}$ | | |
| 3 | <i>a</i> | 32 | $0,0,0$ | | |

Symmetry of special projectionsAlong [001] $p3m1$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$$

Origin at 0,0,z

Along [100] $p2$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$$

Origin at x,0,0

Along [210] $p11m$

$$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \frac{1}{3}\mathbf{c}$$

Origin at $x, \frac{1}{2}x, 0$

R32

D₃⁷

32

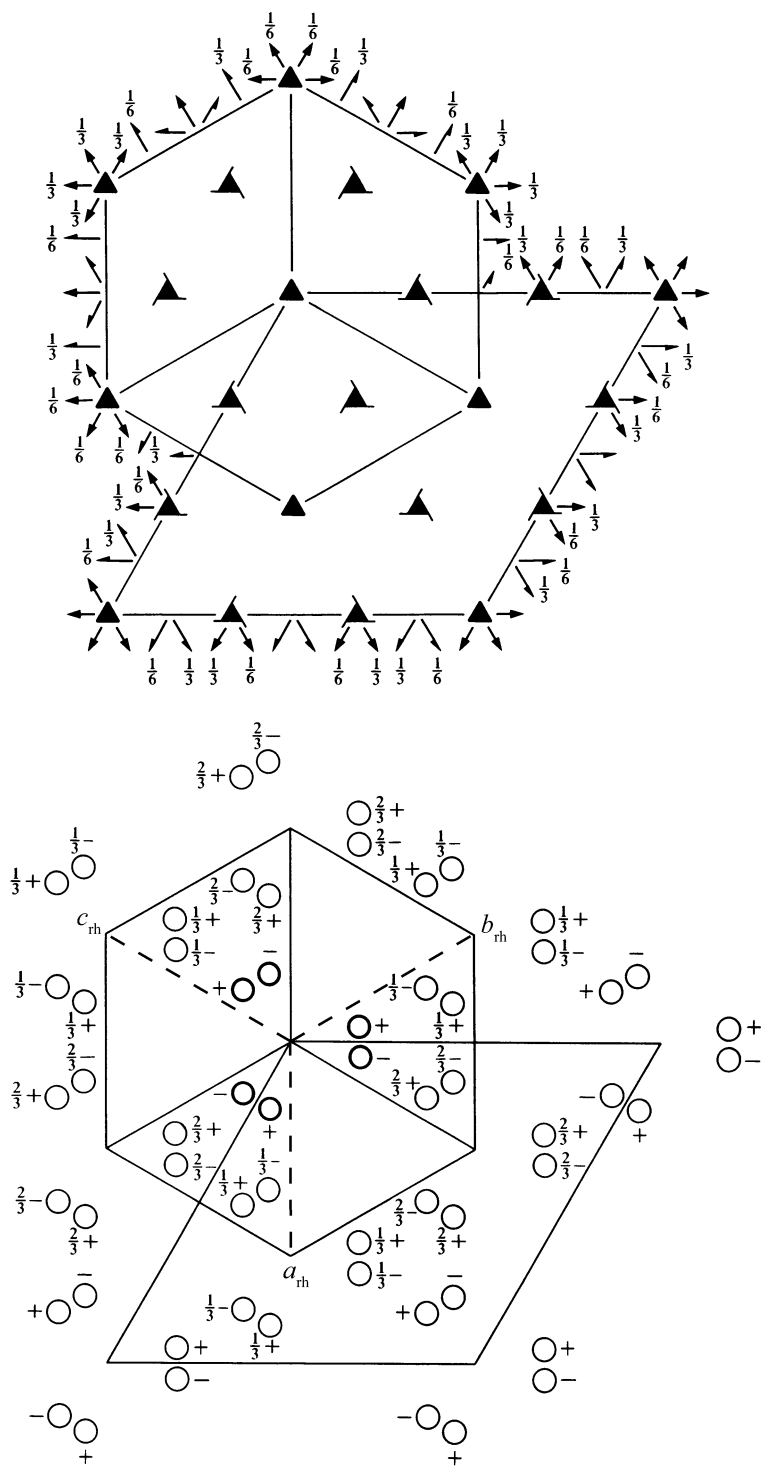
Trigonal

No. 155

R32

Patterson symmetry R $\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin at 32

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

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry operations

- (1) 1 (2) 3^+ x, x, x (3) 3^- x, x, x
 (4) 2 $\bar{x}, 0, x$ (5) 2 $x, \bar{x}, 0$ (6) 2 $0, y, \bar{y}$

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (4)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

- 6 f 1 (1) x, y, z (2) z, x, y (3) y, z, x
 (4) $\bar{z}, \bar{y}, \bar{x}$ (5) $\bar{y}, \bar{x}, \bar{z}$ (6) $\bar{x}, \bar{z}, \bar{y}$

General:

no conditions

Special: no extra conditions

- 3 e .2 $x, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, x, \bar{x}$ $\bar{x}, \frac{1}{2}, x$

- 3 d .2 $x, \bar{x}, 0$ $0, x, \bar{x}$ $\bar{x}, 0, x$

- 2 c 3. x, x, x $\bar{x}, \bar{x}, \bar{x}$

- 1 b 32 $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

- 1 a 32 0, 0, 0

Symmetry of special projections

Along $[111] p3m1$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x

Along $[1\bar{1}0] p2$

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

Origin at $x, \bar{x}, 0$

Along $[2\bar{1}\bar{1}] p11m$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$$

Origin at $2x, \bar{x}, \bar{x}$