

Symmetry operations

For (0,0,0)+ set

- | | | |
|---------------------------|----------------------------------|----------------------------------|
| (1) 1 | (2) $3^+ 0, 0, z$ | (3) $3^- 0, 0, z$ |
| (4) $2 x, x, \frac{1}{4}$ | (5) $2 x, 0, \frac{1}{4}$ | (6) $2 0, y, \frac{1}{4}$ |
| (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) $c x, \bar{x}, z$ | (11) $c x, 2x, z$ | (12) $c 2x, x, z$ |

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) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{6}, \frac{5}{12}$ | (5) $2(\frac{1}{2}, 0, 0) x, \frac{1}{6}, \frac{5}{12}$ | (6) $2 \frac{1}{3}, y, \frac{5}{12}$ |
| (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) $g(\frac{1}{6}, -\frac{1}{6}, \frac{5}{6}) x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{6}, \frac{1}{3}, \frac{5}{6}) x + \frac{1}{4}, 2x, z$ | (12) $g(\frac{2}{3}, \frac{1}{3}, \frac{5}{6}) 2x, x, z$ |

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) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{6}, \frac{1}{12}$ | (5) $2 x, \frac{1}{3}, \frac{1}{12}$ | (6) $2(0, \frac{1}{2}, 0) \frac{1}{6}, y, \frac{1}{12}$ |
| (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) $g(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}) x + \frac{1}{2}, \bar{x}, z$ | (11) $g(\frac{1}{3}, \frac{2}{3}, \frac{1}{6}) x, 2x, z$ | (12) $g(\frac{1}{3}, \frac{1}{6}, \frac{1}{6}) 2x - \frac{1}{2}, x, z$ |

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

Reflection conditions

General:

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

- $hkil: -h + k + l = 3n$
 $hki0: -h + k = 3n$
 $h\bar{h}2hl: l = 3n$
 $h\bar{h}0l: h + l = 3n, l = 2n$
 $000l: l = 6n$
 $h\bar{h}00: h = 3n$

Special: as above, plus

- | | | | | | | | | |
|----|-----|-------------|---------------------|-------------------------------|---------------------------------|-------------------------------|-------------------------------|---|
| 18 | e | . 2 | $x, 0, \frac{1}{4}$ | $0, x, \frac{1}{4}$ | $\bar{x}, \bar{x}, \frac{1}{4}$ | $\bar{x}, 0, \frac{3}{4}$ | $0, \bar{x}, \frac{3}{4}$ | $x, x, \frac{3}{4}$ |
| 18 | d | $\bar{1}$ | $\frac{1}{2}, 0, 0$ | $0, \frac{1}{2}, 0$ | $\frac{1}{2}, \frac{1}{2}, 0$ | $0, \frac{1}{2}, \frac{1}{2}$ | $\frac{1}{2}, 0, \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |
| 12 | c | 3. | $0, 0, z$ | $0, 0, \bar{z} + \frac{1}{2}$ | $0, 0, \bar{z}$ | $0, 0, z + \frac{1}{2}$ | | |
| 6 | b | $\bar{3}$. | $0, 0, 0$ | $0, 0, \frac{1}{2}$ | | | | |
| 6 | a | 3 2 | $0, 0, \frac{1}{4}$ | $0, 0, \frac{3}{4}$ | | | | |

no extra conditions

 $hkil: l = 2n$ $hkil: l = 2n$ $hkil: l = 2n$ $hkil: l = 2n$

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] $p2$ $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} + 4\mathbf{b} + \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$ Origin at $x, 0, 0$ Along [210] $p2gm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

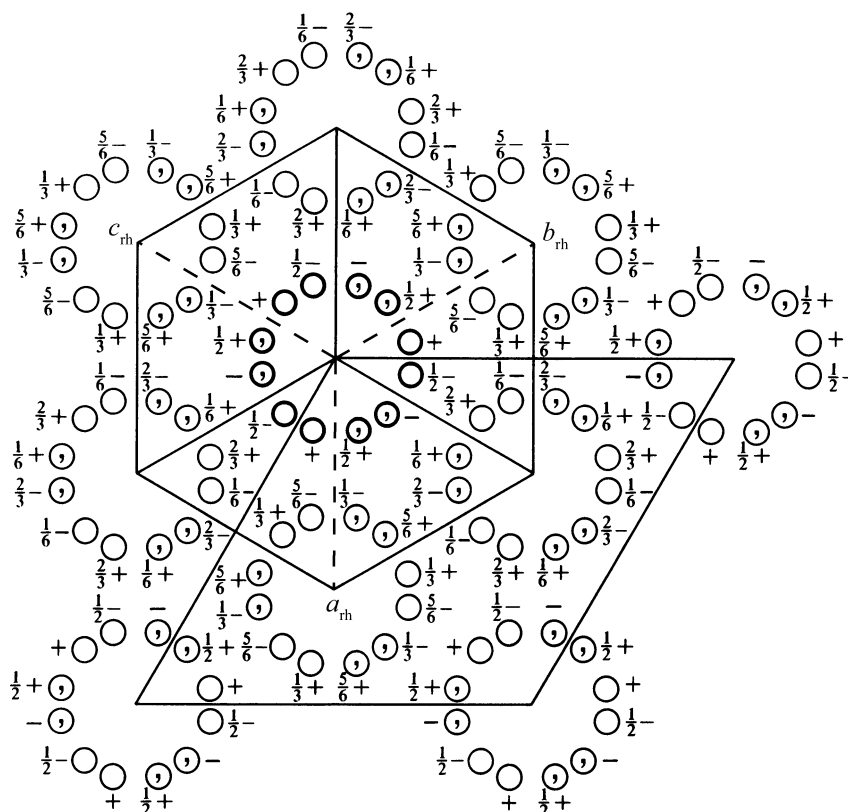
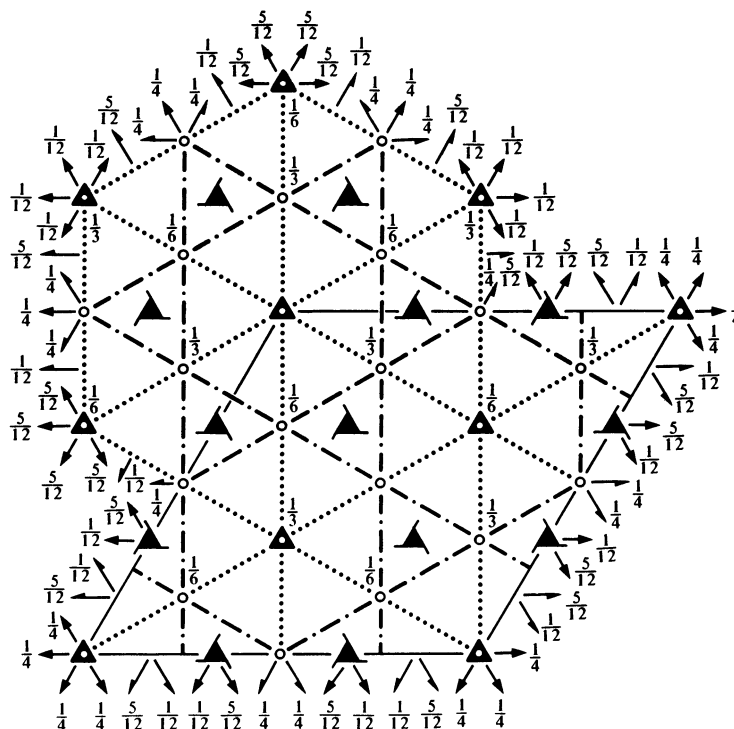
$R\bar{3}c$ D_{3d}^6 $\bar{3}m$

Trigonal

No. 167

 $R\bar{3}2/c$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin $(\bar{3})$ at $\bar{3}c$ Asymmetric unit $\frac{1}{4} \leq x \leq \frac{5}{4}$; $\frac{1}{4} \leq y \leq \frac{5}{4}$; $\frac{1}{4} \leq z \leq \frac{3}{4}$; $y \leq x$; $z \leq \min(y, \frac{3}{2} - x)$ Vertices $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{5}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{5}{4}, \frac{5}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$

Symmetry operations

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

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions			
12 <i>f</i> 1	(1) x, y, z (4) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (10) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	(2) z, x, y (5) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{z}, \bar{x}, \bar{y}$ (11) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(3) y, z, x (6) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (9) $\bar{y}, \bar{z}, \bar{x}$ (12) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	General: $hhl: l = 2n$ $hhh: h = 2n$ Special: as above, plus no extra conditions			
6 <i>e</i> .2	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, x, \bar{x} + \frac{1}{2}$ $\frac{3}{4}, \bar{x}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ $x + \frac{1}{2}, \frac{3}{4}, \bar{x}$				
6 <i>d</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$hkl: h + k + l = 2n$
4 <i>c</i> 3.	x, x, x	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{x}, \bar{x}$	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$			$hkl: h + k + l = 2n$
2 <i>b</i> $\bar{3}$.	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					$hkl: h + k + l = 2n$
2 <i>a</i> 32	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$					$hkl: h + k + l = 2n$

Symmetry of special projections

Along $[111] p6mm$

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

Origin at x, x, x

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

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

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

Along $[2\bar{1}\bar{1}] p2gm$

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

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