

$R3c$

C_{3v}^6

$3m$

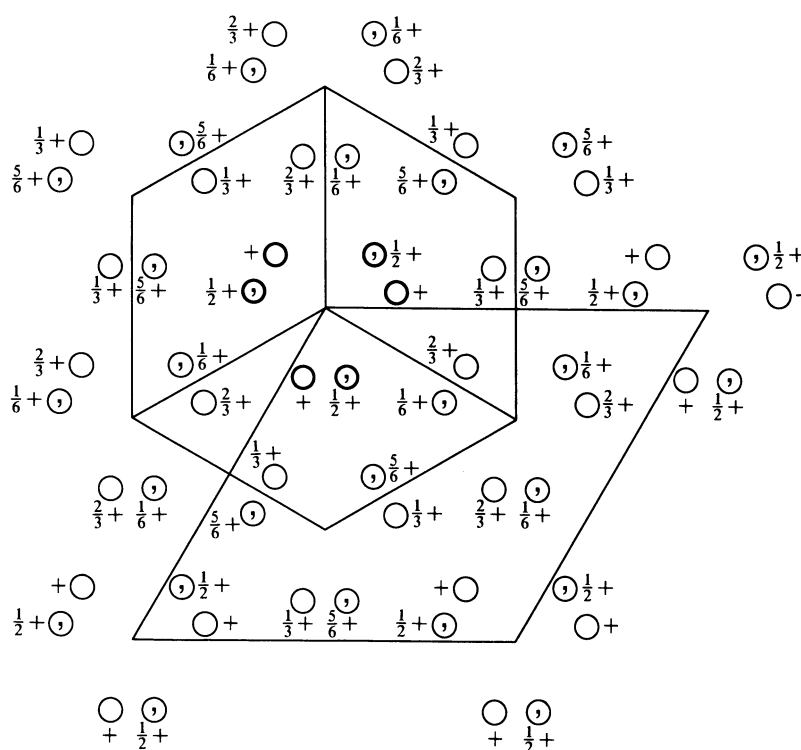
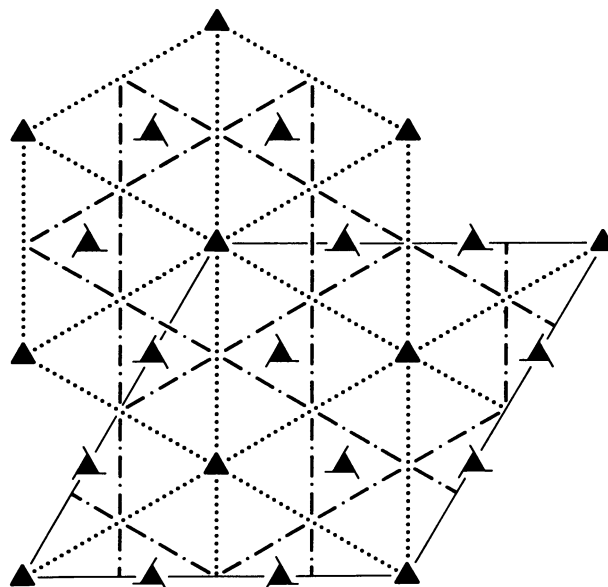
Trigonal

No. 161

$R3c$

Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES



Origin on $3c$

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) $c \ x, \bar{x}, z$ | (5) $c \ x, 2x, z$ | (6) $c \ 2x, x, z$ |

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

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

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)**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>b</i> | 1 | (1) x, y, z | (2) $\bar{y}, x - y, z$ | (3) $\bar{x} + y, \bar{x}, z$ |
| | | | (4) $\bar{y}, \bar{x}, z + \frac{1}{2}$ | (5) $\bar{x} + y, y, z + \frac{1}{2}$ | (6) $x, x - y, z + \frac{1}{2}$ |

Reflection conditions

General:

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

Special: as above, plus

 $hkil: l = 2n$ 6 *a* 3. $0,0,z$ $0,0,z + \frac{1}{2}$ **Symmetry of special projections**Along [001] $p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$

Origin at 0,0,z

Along [100] $p1$ $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} + 4\mathbf{b} + \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$

Origin at x,0,0

Along [210] $p1g1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$

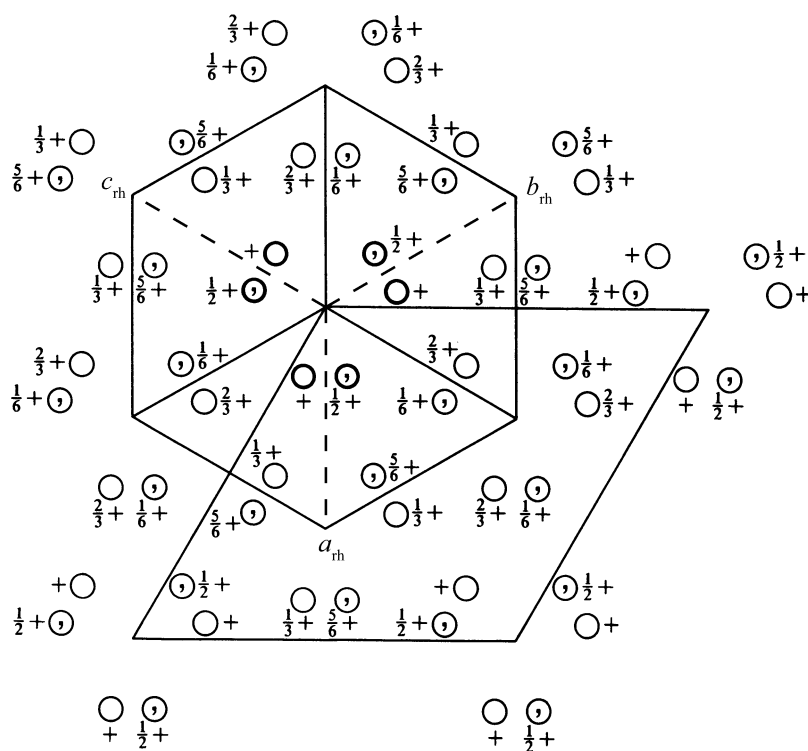
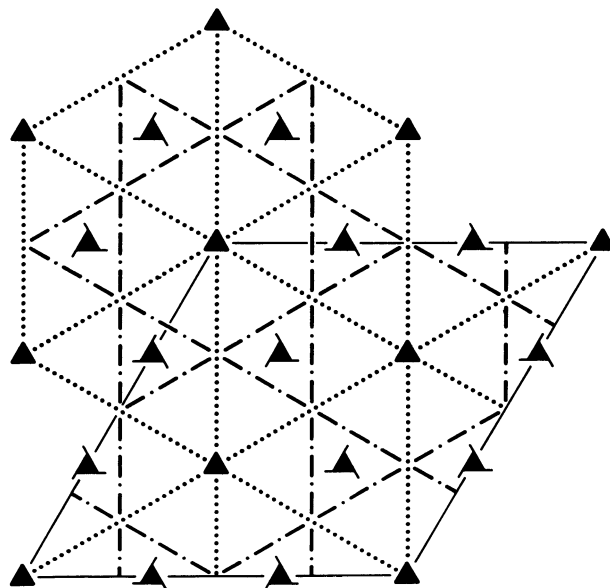
$R3c$ C_{3v}^6 $3m$

Trigonal

No. 161

 $R3c$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin on $3c$ **Asymmetric unit** $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1; y \leq x; z \leq y$ Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 1,1,1$

Symmetry operations

- (1) 1 (2) $3^+ x, x, x$ (3) $3^- x, x, x$
 (4) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, x$ (5) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, x, z$ (6) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y, y$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 <i>b</i> 1	(1) x, y, z (4) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	(2) z, x, y (5) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(3) y, z, x (6) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	General: <i>hhl</i> : $l = 2n$ <i>hhh</i> : $h = 2n$ Special: as above, plus <i>hkl</i> : $h + k + l = 2n$
2 <i>a</i> 3.	x, x, x	$x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$		

Symmetry of special projections

Along $[111] p31m$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ Origin at x, x, x	$\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$	Along $[1\bar{1}0] p1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - 2\mathbf{c})$ Origin at $x, \bar{x}, 0$	$\mathbf{b}' = \frac{1}{2}\mathbf{c}$	Along $[2\bar{1}\bar{1}] p1g1$ $\mathbf{a}' = \frac{1}{2}(\mathbf{b} - \mathbf{c})$ Origin at $2x, \bar{x}, \bar{x}$	$\mathbf{b}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$
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