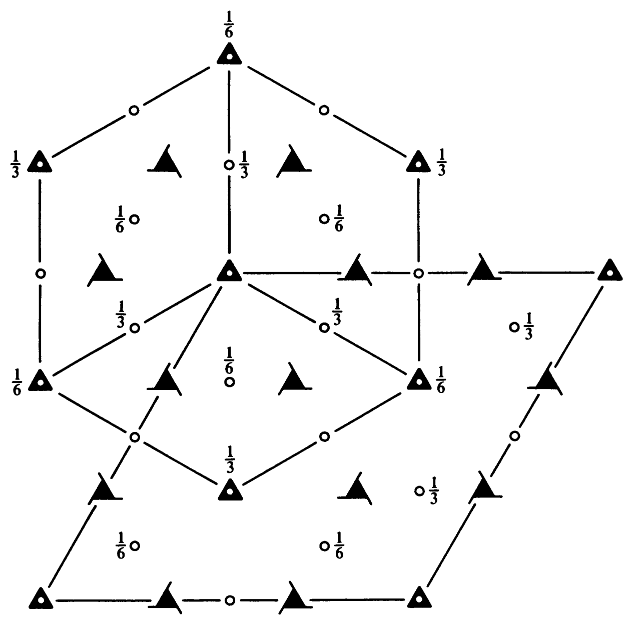
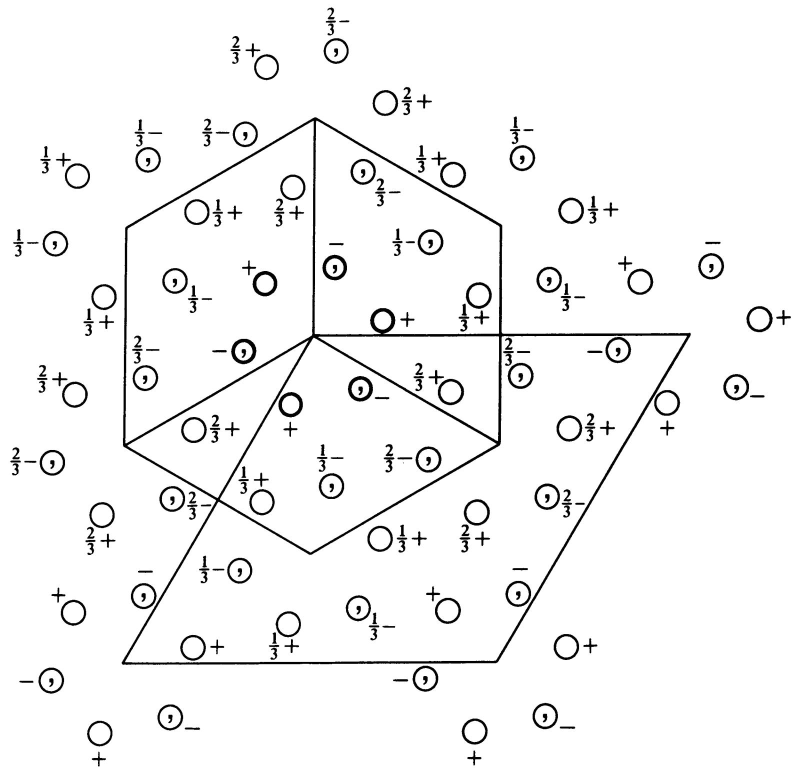
International Tables for Crystallography (2006). Vol. A, Space group 148, pp. 502–503.

$R\bar{3}$ C_{3i}^{2} $\bar{3}$ Trigonal

No. 148 $R\bar{3}$ Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

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

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

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

Symmetry operations

(1) 1 (2) 3^{+} x,x,x (3) 3^{-} x,x,x

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

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
						General:
6	*f*	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
			(4) $\bar{x},\bar{y},\bar{z}$	(5) $\bar{z},\bar{x},\bar{y}$	(6) $\bar{y},\bar{z},\bar{x}$	
						Special: no extra conditions
3	*e*	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	
3	*d*	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	
2	*c*	3 .	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	*b*	$\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	*a*	$\bar{3}$.	$0,0,0$			

Symmetry of special projections

Along [111] $p6$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

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

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

Maximal non-isomorphic subgroups

I [2] $R3$ (146) 1; 2; 3
[3] $R\bar{1}$ ($P\bar{1}$, 2) 1; 4

IIa none

IIb [3] $P\bar{3}$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b}, \mathbf{b}'=\mathbf{b}-\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (147)

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}$ ($\mathbf{a}'=\mathbf{b}+\mathbf{c}, \mathbf{b}'=\mathbf{a}+\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}$) (148); [4] $R\bar{3}$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (148)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $Pm\bar{3}$ (200); [4] $Pn\bar{3}$ (201); [4] $Fm\bar{3}$ (202); [4] $Fd\bar{3}$ (203); [4] $Im\bar{3}$ (204); [4] $Pa\bar{3}$ (205); [4] $Ia\bar{3}$ (206)

II [3] $P\bar{3}$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (147)