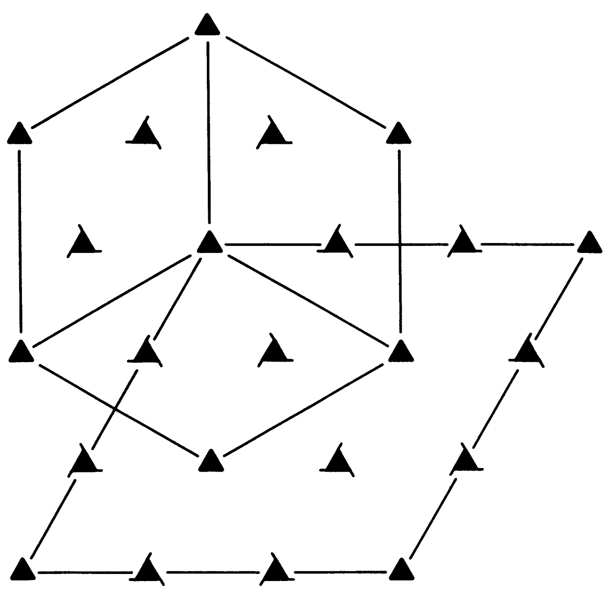
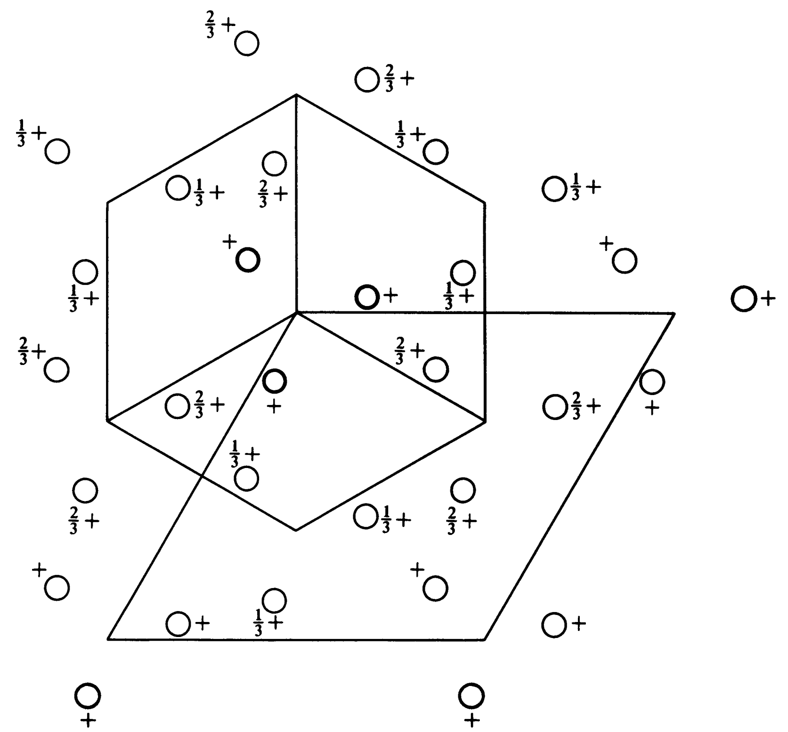
*R*3 C_3^4 3 Trigonal

No. 146 *R*3 Patterson symmetry $R\bar{3}$

HEXAGONAL AXES





Origin on 3

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

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

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

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$

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) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$

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) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$

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)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
9	b	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$ $hki0$: $-h+k=3n$ $hh\overline{2h}l$: $l=3n$ $h\bar{h}0l$: $h+l=3n$ $000l$: $l=3n$ $h\bar{h}00$: $h=3n$
						Special: no extra conditions
3	a	3 .	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [3] $R1$ ($P1$, 1) 1+

IIa [3] $P3_2$ (145) 1; $2+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; $3+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
[3] $P3_1$ (144) 1; $2+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $3+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
[3] $P3$ (143) 1; 2; 3

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $R3$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (146); [4] $R3$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (146)

Minimal non-isomorphic supergroups

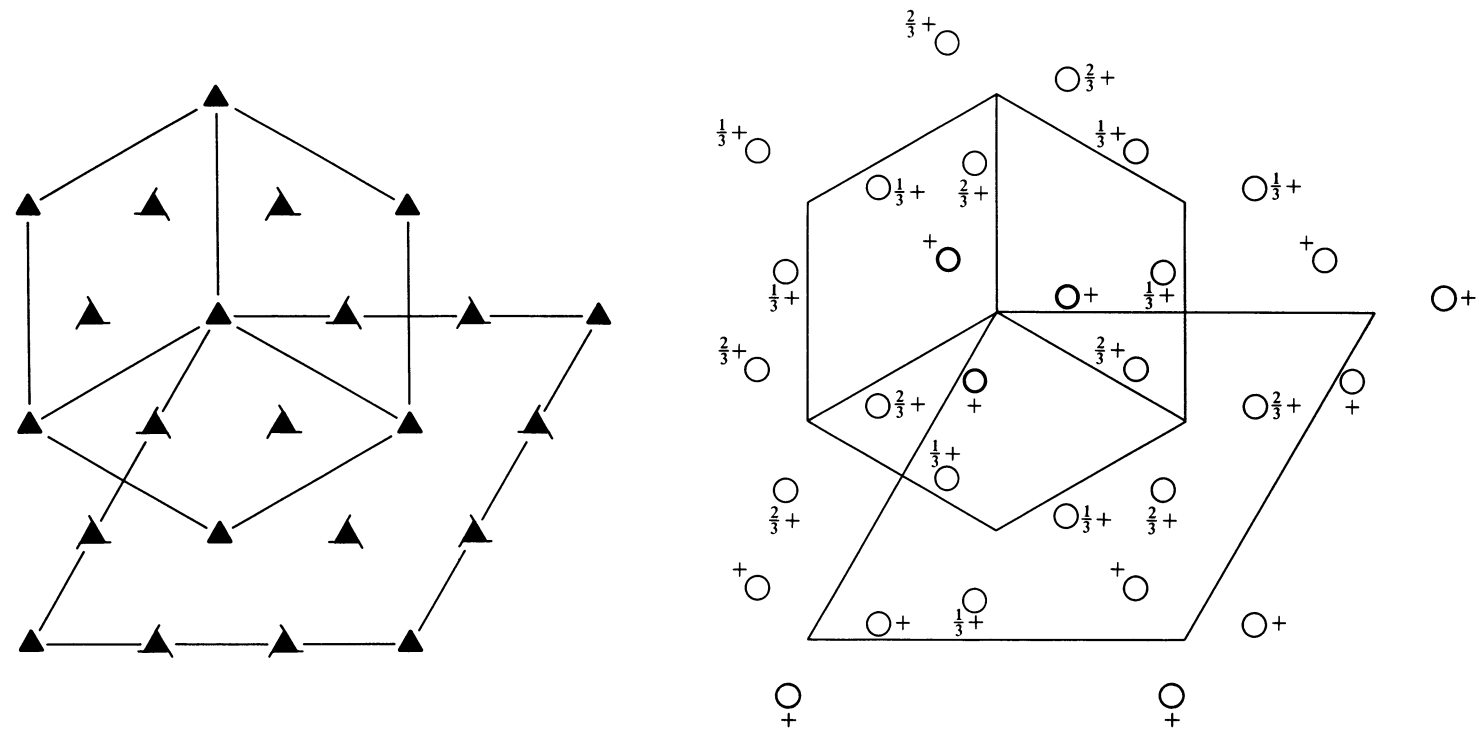
I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)

II [3] $P3$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (143)

$R3$ | C_3^4 | 3 | **Trigonal**

No. 146 | $R3$ | Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin on 3

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le 1$; $z \le \min(x,y)$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$ $1,1,1$

Symmetry operations

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	b	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
						Special: no extra conditions
1	a	3 .	x,x,x			

Symmetry of special projections

Along [111] $p3$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

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

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

Maximal non-isomorphic subgroups

I [3] $R1$ ($P1$, 1) 1

IIa none

IIb [3] $P3_2$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{b}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$) (145); [3] $P3_1$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{b}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$) (144); [3] $P3$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{b}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$) (143)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3$ ($\mathbf{a}' = \mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}$) (146); [4] $R3$ ($\mathbf{a}' = -\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}-\mathbf{c}$) (146)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)

II [3] $P3$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (143)