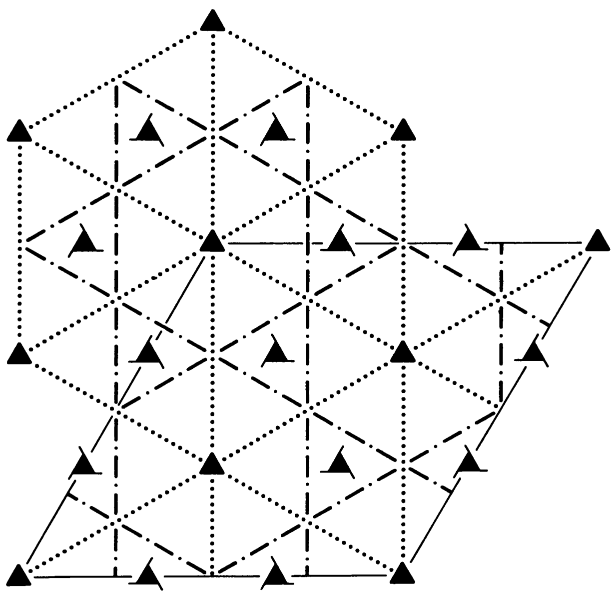
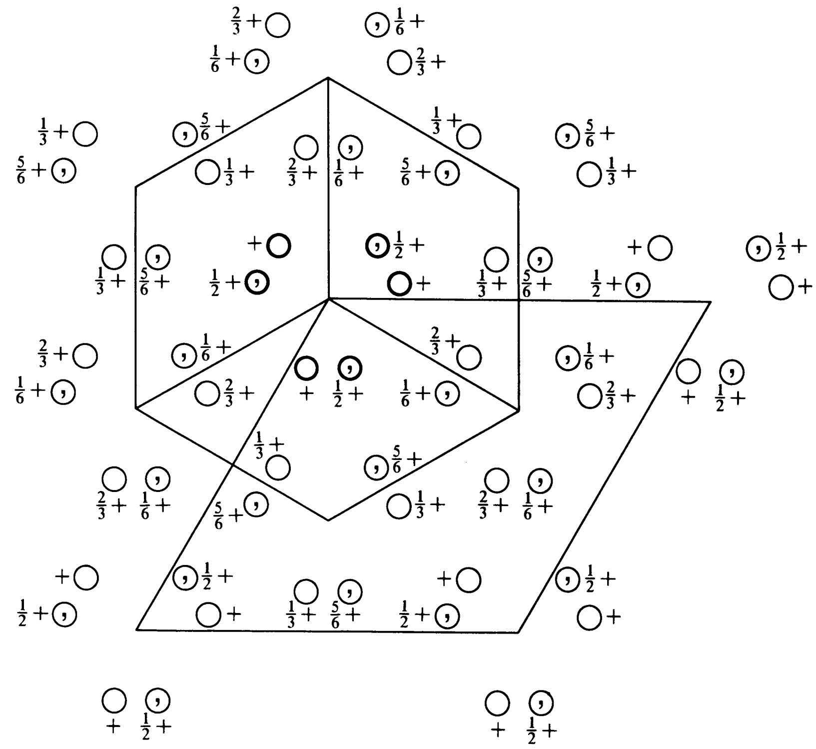
$R3c$ C_{3v}^6 $3m$ Trigonal

No. 161 $R3c$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin on $3c$

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

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

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

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

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

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

General:

Multiplicity	Wyckoff letter	Site symmetry	Coordinates			Reflection conditions
18	b	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
			(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$	$hki0$: $-h+k=3n$
						$hh\overline{2h}l$: $l=3n$
						$h\bar{h}0l$: $h+l=3n$, $l=2n$
						$000l$: $l=6n$
						$h\bar{h}00$: $h=3n$
						Special: as above, plus
6	a	$3.$	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

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

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) (1; 2; 3)+
{ [3] $R1c$ (Cc, 9) (1; 4)+
{ [3] $R1c$ (Cc, 9) (1; 5)+
{ [3] $R1c$ (Cc, 9) (1; 6)+

IIa [3] $P3c1$ (158) 1; 2; 3; 4; 5; 6

IIb none

Maximal isomorphic subgroups of lowest index

IIc [4] $R3c$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (161); [5] $R3c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=5c$) (161)

Minimal non-isomorphic supergroups

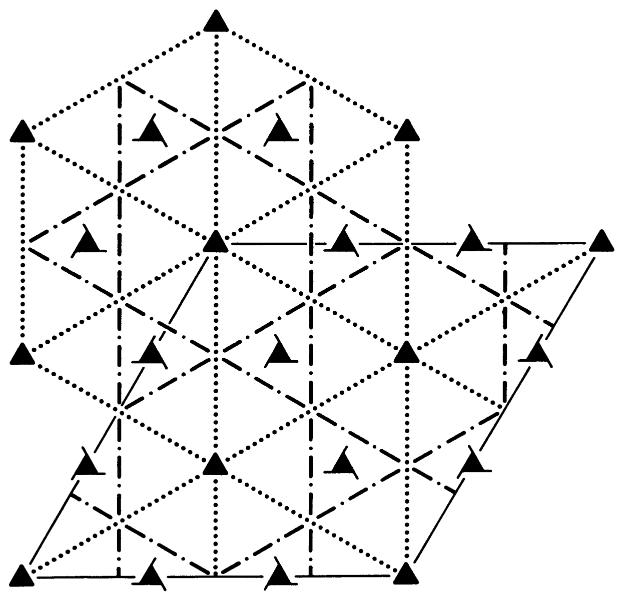
I [2] $R\bar{3}c$ (167); [4] $P\bar{4}3n$ (218); [4] $F\bar{4}3c$ (219); [4] $I\bar{4}3d$ (220)

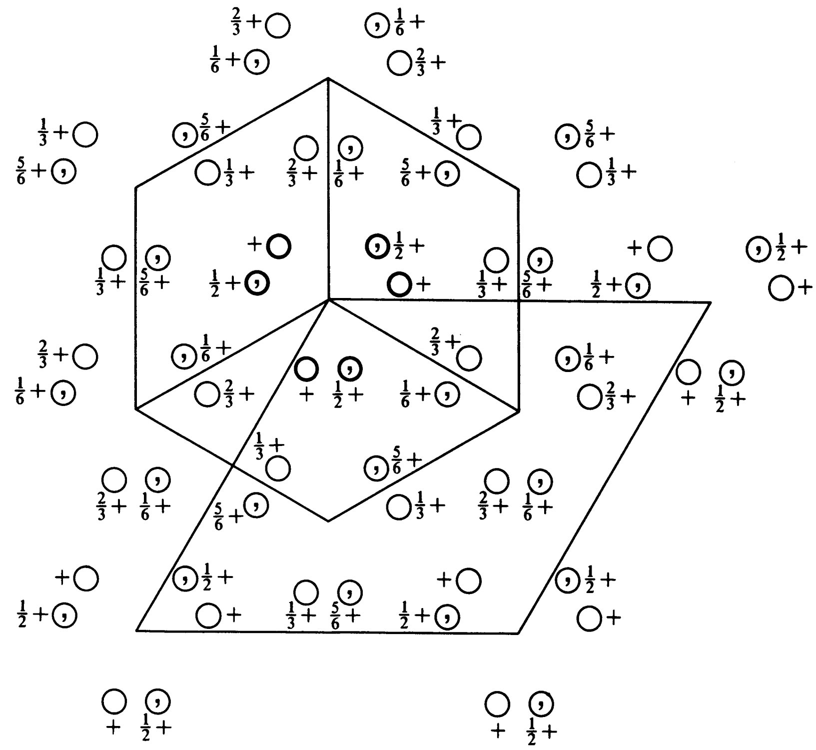
II [2] $R3m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (160); [3] $P31c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (159)

$R3c$ 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 $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le 1$; $y \le x$; $z \le y$

Vertices 0,0,0 1,0,0 1,1,0 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
						General:
6	b	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl : $l=2n$
			(4) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(5) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(6) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	hhh : $h=2n$
						Special: as above, plus
2	a	$3\,.$	x,x,x	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$		hkl : $h+k+l=2n$

Symmetry of special projections

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

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

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

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) 1; 2; 3
{ [3] $R1c$ (Cc, 9) 1; 4
{ [3] $R1c$ (Cc, 9) 1; 5
{ [3] $R1c$ (Cc, 9) 1; 6

IIa none

IIb [3] $P3c1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (158)

Maximal isomorphic subgroups of lowest index

IIc [4] $R3c$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (161); [5] $R3c$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b}+2\mathbf{c},\mathbf{b}'=2\mathbf{a}+\mathbf{b}+2\mathbf{c},\mathbf{c}'=2\mathbf{a}+2\mathbf{b}+\mathbf{c}$) (161)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}c$ (167); [4] $P\bar{4}3n$ (218); [4] $F\bar{4}3c$ (219); [4] $I\bar{4}3d$ (220)

II [2] $R3m$ ($\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\mathbf{b}'=\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\mathbf{c}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$) (160);
[3] $P31c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (159)