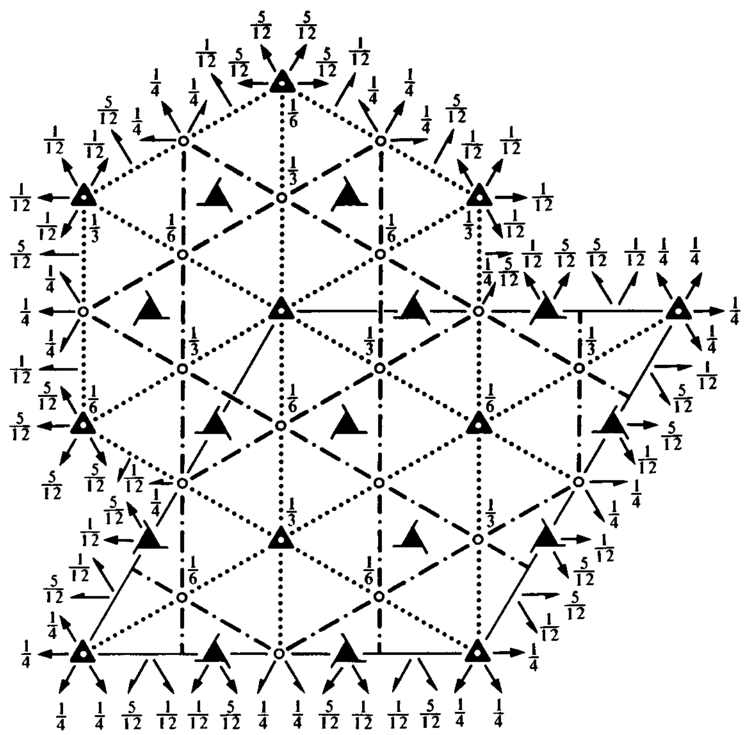
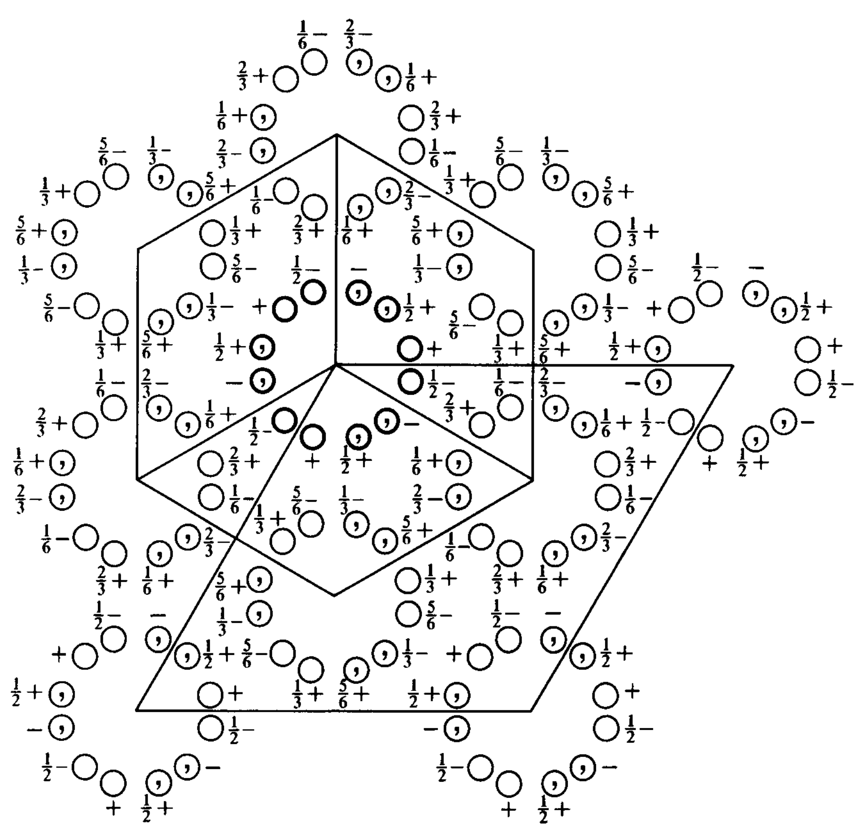
*International Tables for Crystallography* (2006). Vol. A, Space group 167, pp. 548–551.

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

No. 167 $\quad R\bar{3}2/c$ $\quad$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





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

**Asymmetric unit** $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{12};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

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

$0,0,\frac{1}{12} \quad \frac{1}{2},0,\frac{1}{12} \quad \frac{2}{3},\frac{1}{3},\frac{1}{12} \quad \frac{1}{3},\frac{2}{3},\frac{1}{12} \quad 0,\frac{1}{2},\frac{1}{12}$

## 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

| Multiplicity | Wyckoff letter | Site symmetry | Coordinates | | | | | | Reflection conditions |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | General: |
| 36 | $f$ | $1$ | (1) $x,y,z$ | (2) $\bar{y},x-y,z$ | (3) $\bar{x}+y,\bar{x},z$ | | | | $hkil$ : $-h+k+l=3n$ |
| | | | (4) $y,x,\bar{z}+\frac{1}{2}$ | (5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ | (6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ | | | | $hki0$ : $-h+k=3n$ |
| | | | (7) $\bar{x},\bar{y},\bar{z}$ | (8) $y,\bar{x}+y,\bar{z}$ | (9) $x-y,x,\bar{z}$ | | | | $hh\overline{2h}l$ : $l=3n$ |
| | | | (10) $\bar{y},\bar{x},z+\frac{1}{2}$ | (11) $\bar{x}+y,y,z+\frac{1}{2}$ | (12) $x,x-y,z+\frac{1}{2}$ | | | | $h\bar{h}0l$ : $h+l=3n,\ l=2n$ |
| | | | | | | | | | $000l$ : $l=6n$ |
| | | | | | | | | | $h\bar{h}00$ : $h=3n$ |
| | | | | | | | | | Special: as above, plus |
| 18 | $e$ | $.2$ | $x,0,\frac{1}{4}$ | $0,x,\frac{1}{4}$ | $\bar{x},\bar{x},\frac{1}{4}$ | $\bar{x},0,\frac{3}{4}$ | $0,\bar{x},\frac{3}{4}$ | $x,x,\frac{3}{4}$ | no extra conditions |
| 18 | $d$ | $\bar{1}$ | $\frac{1}{2},0,0$ | $0,\frac{1}{2},0$ | $\frac{1}{2},\frac{1}{2},0$ | $0,\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},0,\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | $hkil$ : $l=2n$ |
| 12 | $c$ | $3.$ | $0,0,z$ | $0,0,\bar{z}+\frac{1}{2}$ | $0,0,\bar{z}$ | $0,0,z+\frac{1}{2}$ | | | $hkil$ : $l=2n$ |
| 6 | $b$ | $\bar{3}.$ | $0,0,0$ | $0,0,\frac{1}{2}$ | | | | | $hkil$ : $l=2n$ |
| 6 | $a$ | $32$ | $0,0,\frac{1}{4}$ | $0,0,\frac{3}{4}$ | | | | | $hkil$ : $l=2n$ |

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

HEXAGONAL AXES

**Maximal non-isomorphic subgroups**

**I** [2] $R3c$ (161) (1; 2; 3; 10; 11; 12)+
[2] $R32$ (155) (1; 2; 3; 4; 5; 6)+
[2] $R\bar{3}1$ ($R\bar{3}$, 148) (1; 2; 3; 7; 8; 9)+
{ [3] $R12/c$ ($C2/c$, 15) (1; 4; 7; 10)+
[3] $R12/c$ ($C2/c$, 15) (1; 5; 7; 11)+
[3] $R12/c$ ($C2/c$, 15) (1; 6; 7; 12)+ }

**IIa** { [3] $P\bar{3}c1$ (165) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $P\bar{3}c1$ (165) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
[3] $P\bar{3}c1$ (165) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ }

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [4] $R\bar{3}c$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=5\mathbf{c}$) (167)

**Minimal non-isomorphic supergroups**

**I** [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

**II** [2] $R\bar{3}m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (166); [3] $P\bar{3}1c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (163)

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RHOMBOHEDRAL AXES

**Maximal non-isomorphic subgroups**

**I** [2] $R3c$ (161) 1; 2; 3; 10; 11; 12
[2] $R32$ (155) 1; 2; 3; 4; 5; 6
[2] $R\bar{3}1$ ($R\bar{3}$, 148) 1; 2; 3; 7; 8; 9
{ [3] $R12/c$ ($C2/c$, 15) 1; 4; 7; 10
[3] $R12/c$ ($C2/c$, 15) 1; 5; 7; 11
[3] $R12/c$ ($C2/c$, 15) 1; 6; 7; 12 }

**IIa** none

**IIb** [3] $P\bar{3}c1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (165)

**Maximal isomorphic subgroups of lowest index**

**IIc** [4] $R\bar{3}c$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b}+2\mathbf{c},\mathbf{b}'=2\mathbf{a}+\mathbf{b}+2\mathbf{c},\mathbf{c}'=2\mathbf{a}+2\mathbf{b}+\mathbf{c}$) (167)

**Minimal non-isomorphic supergroups**

**I** [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

**II** [2] $R\bar{3}m$ ($\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\mathbf{b}'=\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\mathbf{c}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$) (166);
[3] $P\bar{3}1c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (163)

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

Patterson symmetry $R\bar{3}m$ $R\bar{3}2/c$ No. 167

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

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

**Asymmetric unit** $\frac{1}{4} \le x \le \frac{5}{4}$; $\frac{1}{4} \le y \le \frac{5}{4}$; $\frac{1}{4} \le z \le \frac{3}{4}$; $y \le x$; $z \le \min(y, \frac{3}{2} - x)$

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) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $x,x,z$ | (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 |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | General: |
| 12 | $f$ | $1$ | (1) $x,y,z$ | (2) $z,x,y$ | (3) $y,z,x$ | | | | $hhl$ : $l=2n$ |
| | | | (4) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$ | (5) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ | (6) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ | | | | $hhh$ : $h=2n$ |
| | | | (7) $\bar{x},\bar{y},\bar{z}$ | (8) $\bar{z},\bar{x},\bar{y}$ | (9) $\bar{y},\bar{z},\bar{x}$ | | | | |
| | | | (10) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$ | (11) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ | (12) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ | | | | |
| | | | | | | | | | Special: as above, plus |
| 6 | $e$ | $.2$ | $x,\bar{x}+\frac{1}{2},\frac{1}{4}$ | $\frac{1}{4},x,\bar{x}+\frac{1}{2}$ | $\bar{x}+\frac{1}{2},\frac{1}{4},x$ | | | | no extra conditions |
| | | | $\bar{x},x+\frac{1}{2},\frac{3}{4}$ | $\frac{3}{4},\bar{x},x+\frac{1}{2}$ | $x+\frac{1}{2},\frac{3}{4},\bar{x}$ | | | | |
| 6 | $d$ | $\bar{1}$ | $\frac{1}{2},0,0$ | $0,\frac{1}{2},0$ | $0,0,\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},0$ | $\frac{1}{2},0,\frac{1}{2}$ | $0,\frac{1}{2},\frac{1}{2}$ | $hkl$ : $h+k+l=2n$ |
| 4 | $c$ | $3.$ | $x,x,x$ | $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ | $\bar{x},\bar{x},\bar{x}$ | $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ | | | $hkl$ : $h+k+l=2n$ |
| 2 | $b$ | $\bar{3}.$ | $0,0,0$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | | | | | $hkl$ : $h+k+l=2n$ |
| 2 | $a$ | $32$ | $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ | | | | | $hkl$ : $h+k+l=2n$ |

**Symmetry of special projections**

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at $x,x,x$

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

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

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