International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 167, pp. 314–316.

$R\bar{3}c$ No. 167 $R\bar{3}2/c$ D_{3d}^6

HEXAGONAL AXES

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)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
	$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
36 f 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
	(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$
	(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
	(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $R3c$ (161)	(1; 2; 3; 10; 11; 12)+		
[2] $R32$ (155)	(1; 2; 3; 4; 5; 6)+		$0,0,1/4$
[2] $R\bar{3}1$ (148, $R\bar{3}$)	(1; 2; 3; 7; 8; 9)+		
[3] $R12/c$ (15, $C12/c1$)	(1; 4; 7; 10)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $R12/c$ (15, $C12/c1$)	(1; 5; 7; 11)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$	
[3] $R12/c$ (15, $C12/c1$)	(1; 6; 7; 12)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

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

- **Enlarged unit cell**

[4] $\mathbf{a}'=-2\mathbf{b},\ \mathbf{b}'=2\mathbf{a}+2\mathbf{b}$

$R\bar{3}c$ (167)	$\langle 2;\ 4;\ 7\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$R\bar{3}c$ (167)	$\langle(2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$R\bar{3}c$ (167)	$\langle 2+(1,2,0);\ 4+(-1,1,0);\ 7+(0,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
$R\bar{3}c$ (167)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 5\ (\mathrm{mod}\ 6)$	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	$0,0,u$
$R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\ (\mathrm{mod}\ 6)$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=-p\mathbf{b},\ \mathbf{b}'=p\mathbf{a}+p\mathbf{b}$

$R\bar{3}c$ (167)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);\ 7+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2\ (\mathrm{mod}\ 3)$	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$R\bar{3}c$ (167)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);\ 7+(2u,2v,0)\rangle$ $p>6;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1\ (\mathrm{mod}\ 3)$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[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 Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

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

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 f 1	(1) x,y,z	(2) z,x,y	(3) y,z,x
	(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) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$
	(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) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $R3c$ (161)	1; 2; 3; 10; 11; 12		
[2] $R32$ (155)	1; 2; 3; 4; 5; 6		$1/4,1/4,1/4$
[2] $R\bar{3}1$ (148, $R\bar{3}$)	1; 2; 3; 7; 8; 9		
[3] $R12/c$ (15, $C12/c1$)	1; 4; 7; 10	$-\mathbf{a}-\mathbf{c},-\mathbf{a}+\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[3] $R12/c$ (15, $C12/c1$)	1; 5; 7; 11	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[3] $R12/c$ (15, $C12/c1$)	1; 6; 7; 12	$-\mathbf{b}-\mathbf{c},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{b}-\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$

$P\bar{3}c1$ (165)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
$P\bar{3}c1$ (165)	$\langle 2+(1,-1,0);\ 4+(1,0,1);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,0$
$P\bar{3}c1$ (165)	$\langle 2+(1,0,-1);\ 4+(1,2,1);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,1,0$

[4] $\mathbf{a}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}$

$R\bar{3}c$ (167)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	
$R\bar{3}c$ (167)	$\langle (2;\ 4)+(1,-2,1);\ 7+(2,-2,0)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,-1,0$
$R\bar{3}c$ (167)	$\langle 2+(1,1,-2);\ 4+(-1,2,-1);\ 7+(0,2,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1,-1$
$R\bar{3}c$ (167)	$\langle 4;\ 2+(2,-1,-1);\ 7+(2,0,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,-1$

- **Series of maximal isomorphic subgroups**

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

$R\bar{3}c$ (167)	$\langle 2;\ 4+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u);$ $7+(2u,2u,2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 5\pmod 6$	$\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations	u,u,u

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

$R\bar{3}c$ (167)	$\langle 2;\ 4+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u);$ $7+(2u,2u,2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\pmod 6$	$\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations	u,u,u

[p^2] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}c$ (167)	$\langle 2+(u+v,-2u+v,u-2v);$ $4+(u-v,-2u+2v,u-v);$ $7+(2u,-2u+2v,-2v)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2\pmod 3$	$\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations	$u,-u+v,-v$

[p^2] $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}+(1-p)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((1-p)\mathbf{a}+(2p+1)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-p)\mathbf{a}+(1-p)\mathbf{b}+(2p+1)\mathbf{c}\big)$

$R\bar{3}c$ (167)	$\langle 2+(u+v,-2u+v,u-2v);$ $4+(u-v,-2u+2v,u-v);$ $7+(2u,-2u+2v,-2v)\rangle$ $p>6;\ p\equiv 1\pmod 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1\pmod 3$	$\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}\ldots$, see lattice relations	$u,-u+v,-v$

I Minimal *translationengleiche* supergroups

[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 Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

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