

D_{3d}^5
 $R\bar{3}2/m$

No. 166

 $R\bar{3}m$

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	<i>i</i>	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) y,x,\bar{z}	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$
			(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	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$

I Maximal translationengleiche subgroups

[2] $R\bar{3}m$ (160)	(1; 2; 3; 10; 11; 12)+	
[2] $R\bar{3}2$ (155)	(1; 2; 3; 4; 5; 6)+	
[2] $R\bar{3}1$ (148, $R\bar{3}$)	(1; 2; 3; 7; 8; 9)+	
{ [3] $R12/m$ (12, $C12/m1$)	(1; 4; 7; 10)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	(1; 5; 7; 11)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	(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] $P\bar{3}m1$ (164)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12	
{ [3] $P\bar{3}m1$ (164)	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] $P\bar{3}m1$ (164)	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

[2] $\mathbf{a}' = -\mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
$R\bar{3}m$ (166)	$\langle 2; 4; 7 \rangle$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$
$R\bar{3}m$ (166)	$\langle 2; (4; 7) + (0,0,1) \rangle$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$
[2] $\mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$		
$R\bar{3}c$ (167)	$\langle 2; 7; 4 + (0,0,1) \rangle$	$\mathbf{a} + \mathbf{b}, -\mathbf{a}, 2\mathbf{c}$
$R\bar{3}c$ (167)	$\langle 2; 4; 7 + (0,0,1) \rangle$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$
[4] $\mathbf{a}' = -2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$		
$R\bar{3}m$ (166)	$\langle 2; 4; 7 \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
$R\bar{3}m$ (166)	$\langle (2; 4) + (1, -1, 0); 7 + (2, 0, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
$R\bar{3}m$ (166)	$\langle 2 + (1, 2, 0); 4 + (-1, 1, 0); 7 + (0, 2, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
$R\bar{3}m$ (166)	$\langle 4; 2 + (2, 1, 0); 7 + (2, 2, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$

• Series of maximal isomorphic subgroups

[p] $\mathbf{c}' = p\mathbf{c}$		
$R\bar{3}m$ (166)	$\langle 2; (4; 7) + (0,0,2u) \rangle$ $p > 4; 0 \leq u < p$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, p\mathbf{c}$
	p conjugate subgroups for prime $p \equiv 2 \pmod{3}$	
$R\bar{3}m$ (166)	$\langle 2; (4; 7) + (0,0,2u) \rangle$ $p > 6; 0 \leq u < p$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	p conjugate subgroups for prime $p \equiv 1 \pmod{3}$	
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$		
$R\bar{3}m$ (166)	$\langle 2 + (u+v, -u+2v, 0); 4 + (u-v, -u+v, 0); 7 + (2u, 2v, 0) \rangle$ $p > 6; 0 \leq u < p; 0 \leq v < p$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$
	p^2 conjugate subgroups for prime $p \equiv 1 \pmod{3}$	
[p^2] $\mathbf{a}' = -p\mathbf{b}, \mathbf{b}' = p\mathbf{a} + p\mathbf{b}$		
$R\bar{3}m$ (166)	$\langle 2 + (u+v, -u+2v, 0); 4 + (u-v, -u+v, 0); 7 + (2u, 2v, 0) \rangle$ $p > 1; 0 \leq u < p; 0 \leq v < p$	$-p\mathbf{b}, p\mathbf{a} + p\mathbf{b}, \mathbf{c}$
	p^2 conjugate subgroups for prime $p \equiv 2 \pmod{3}$	

I Minimal translationengleiche supergroups

[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

none

- Decreased unit cell

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$, $\mathbf{c}' = \frac{1}{3}\mathbf{c}$ $P\bar{3}1m$ (162)

I Minimal translationengleiche supergroups

[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

none

- Decreased unit cell

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ $P\bar{3}1m$ (162)

RHOMBOHEDRAL AXES

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

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

12	<i>i</i>	1	(1) x, y, z	(2) z, x, y	(3) y, z, x
			(4) $\bar{z}, \bar{y}, \bar{x}$	(5) $\bar{y}, \bar{x}, \bar{z}$	(6) $\bar{x}, \bar{z}, \bar{y}$
			(7) $\bar{x}, \bar{y}, \bar{z}$	(8) $\bar{z}, \bar{x}, \bar{y}$	(9) $\bar{y}, \bar{z}, \bar{x}$
			(10) z, y, x	(11) y, x, z	(12) x, z, y

I Maximal translationengleiche subgroups

[2] $R\bar{3}m$ (160)	1; 2; 3; 10; 11; 12	
[2] $R\bar{3}2$ (155)	1; 2; 3; 4; 5; 6	
[2] $R\bar{3}1$ (148, $R\bar{3}$)	1; 2; 3; 7; 8; 9	
{ [3] $R12/m$ (12, $C12/m1$)	1; 4; 7; 10	$-\mathbf{a} - \mathbf{c}, -\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	1; 5; 7; 11	$-\mathbf{a} - \mathbf{b}, \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b} + \mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	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**

[2] $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{b} + \mathbf{c}$		
$R\bar{3}m$ (166)	$\langle 2; 4; 7 \rangle$	$\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}$
$R\bar{3}m$ (166)	$\langle 2; (4; 7) + (1, 1, 1) \rangle$	$\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}$ 1/2, 1/2, 1/2
[2] $\mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$		
$R\bar{3}c$ (167)	$\langle 2; 7; 4 + (1, 1, 1) \rangle$	$\mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{c}$
$R\bar{3}c$ (167)	$\langle 2; 4; 7 + (1, 1, 1) \rangle$	$\mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{c}$ 1/2, 1/2, 1/2
[3] $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$		
{ $P\bar{3}m1$ (164)	$\langle 2; 4; 7 \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$
{ $P\bar{3}m1$ (164)	$\langle 2 + (1, -1, 0); 4 + (1, 0, 1); 7 + (2, 0, 0) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$ 1, 0, 0
{ $P\bar{3}m1$ (164)	$\langle 2 + (1, 0, -1); 4 + (1, 2, 1); 7 + (2, 2, 0) \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$ 1, 1, 0
[4] $\mathbf{a}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{b} - \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}$		
{ $R\bar{3}m$ (166)	$\langle 2; 4; 7 \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$
{ $R\bar{3}m$ (166)	$\langle (2; 4) + (1, -2, 1); 7 + (2, -2, 0) \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$ 1, -1, 0
{ $R\bar{3}m$ (166)	$\langle 2 + (1, 1, -2); 4 + (-1, 2, -1); 7 + (0, 2, -2) \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$ 0, 1, -1
{ $R\bar{3}m$ (166)	$\langle 4; 2 + (2, -1, -1); 7 + (2, 0, -2) \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$ 1, 0, -1

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} + (p-2)\mathbf{b} + (p+1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p+1)\mathbf{a} + (p+1)\mathbf{b} + (p-2)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((p-2)\mathbf{a} + (p+1)\mathbf{b} + (p+1)\mathbf{c})$		
$R\bar{3}m$ (166)	$\langle 2; (4; 7) + (2u, 2u, 2u) \rangle$	$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations}$
	$p > 4; 0 \leq u < p$	u, u, u
	p conjugate subgroups for prime $p \equiv 2 \pmod{3}$	
[p] $\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} + (p-1)\mathbf{b} + (p-1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p-1)\mathbf{a} + (p+2)\mathbf{b} + (p-1)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((p-1)\mathbf{a} + (p-1)\mathbf{b} + (p+2)\mathbf{c})$		
$R\bar{3}m$ (166)	$\langle 2; (4; 7) + (2u, 2u, 2u) \rangle$	$\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} \dots, \text{see lattice relations}$
	$p > 6; 0 \leq u < p$	u, u, u
	p conjugate subgroups for prime $p \equiv 1 \pmod{3}$	
[p^2] $\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} + (1-2p)\mathbf{b} + (p+1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p+1)\mathbf{a} + (p+1)\mathbf{b} + (1-2p)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((1-2p)\mathbf{a} + (p+1)\mathbf{b} + (p+1)\mathbf{c})$		
$R\bar{3}m$ (166)	$\langle 2 + (u+v, -2u+v, u-2v);$	$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations}$
	$4 + (u-v, -2u+2v, u-v); 7 + (2u, -2u+2v, -2v) \rangle$	$u, -u+v, -v$
	$p > 1; 0 \leq u < p; 0 \leq v < p$	
	p^2 conjugate subgroups for prime $p \equiv 2 \pmod{3}$	
[p^2] $\mathbf{a}' = \frac{1}{3}((2p+1)\mathbf{a} + (1-p)\mathbf{b} + (1-p)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((1-p)\mathbf{a} + (2p+1)\mathbf{b} + (1-p)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((1-p)\mathbf{a} + (1-p)\mathbf{b} + (2p+1)\mathbf{c})$		
$R\bar{3}m$ (166)	$\langle 2 + (u+v, -2u+v, u-2v);$	$\mathbf{a}' = \frac{1}{3}((2p+1)\mathbf{a} \dots, \text{see lattice relations}$
	$4 + (u-v, -2u+2v, u-v); 7 + (2u, -2u+2v, -2v) \rangle$	$u, -u+v, -v$
	$p > 6; 0 \leq u < p; 0 \leq v < p$	
	p^2 conjugate subgroups for prime $p \equiv 1 \pmod{3}$	

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I Minimal translationengleiche supergroups

[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

none

- Decreased unit cell

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$, $\mathbf{c}' = \frac{1}{3}\mathbf{c}$ $P\bar{3}1m$ (162)

I Minimal translationengleiche supergroups

[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

none

- Decreased unit cell

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ $P\bar{3}1m$ (162)