

$R3m$

No. 160

$R3m$

$C_{3v}^5$

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)

General position

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

18 c 1

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

(1)  $x, y, z$  (2)  $\bar{y}, x-y, z$  (3)  $\bar{x}+y, \bar{x}, z$   
(4)  $\bar{y}, \bar{x}, z$  (5)  $\bar{x}+y, y, z$  (6)  $x, x-y, z$

I Maximal translationengleiche subgroups

[2] $R31$ (146, $R3$ )	$\langle 1; 2; 3 \rangle +$	
{ [3] $R1m$ (8, $C1m1$ )	$\langle 1; 4 \rangle +$	$1/3(-\mathbf{a} + \mathbf{b} - 2\mathbf{c}), -\mathbf{a} - \mathbf{b}, \mathbf{c}$
[3] $R1m$ (8, $C1m1$ )	$\langle 1; 5 \rangle +$	$1/3(-\mathbf{a} - 2\mathbf{b} - 2\mathbf{c}), \mathbf{a}, \mathbf{c}$
[3] $R1m$ (8, $C1m1$ )	$\langle 1; 6 \rangle +$	$1/3(2\mathbf{a} + \mathbf{b} - 2\mathbf{c}), \mathbf{b}, \mathbf{c}$

II Maximal klassengleiche subgroups

• Loss of centring translations

[3]  $P3m1$  (156) 1; 2; 3; 4; 5; 6

• Enlarged unit cell

[2] $\mathbf{a}' = -\mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{c}$	$R3m$ (160) $\langle 2; 4 \rangle$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$
[2] $\mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$	$R3c$ (161) $\langle 2; 4 + (0,0,1) \rangle$	$\mathbf{a} + \mathbf{b}, -\mathbf{a}, 2\mathbf{c}$
[4] $\mathbf{a}' = -2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$	$R3m$ (160) $\langle 2; 4 \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
	$R3m$ (160) $\langle 2 + (1, -1, 0); 4 + (1, 1, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ 1, 0, 0
	$R3m$ (160) $\langle 2 + (1, 2, 0); 4 + (1, 1, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ 0, 1, 0
	$R3m$ (160) $\langle 2 + (2, 1, 0); 4 + (2, 2, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ 1, 1, 0

• Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$	$R3m$ (160) $\langle 2; 4 \rangle$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, p\mathbf{c}$
	$p > 1; p \equiv 2 \pmod{3}$	
	no conjugate subgroups	
	$R3m$ (160) $\langle 2; 4 \rangle$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$p > 6; p \equiv 1 \pmod{3}$	
	no conjugate subgroups	
[ $p^2$ ] $\mathbf{a}' = -p\mathbf{b}, \mathbf{b}' = p\mathbf{a} + p\mathbf{b}$	$R3m$ (160) $\langle 2 + (u+v, -u+2v, 0); 4 + (u+v, u+v, 0) \rangle$	$-p\mathbf{b}, p\mathbf{a} + p\mathbf{b}, \mathbf{c}$ $u, v, 0$
	$p > 1; 0 \leq u < p; 0 \leq v < p$	
	$p^2$ conjugate subgroups for prime $p \equiv 2 \pmod{3}$	
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$	$R3m$ (160) $\langle 2 + (u+v, -u+2v, 0); 4 + (u+v, u+v, 0) \rangle$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $u, v, 0$
	$p > 6; 0 \leq u < p; 0 \leq v < p$	
	$p^2$ conjugate subgroups for prime $p \equiv 1 \pmod{3}$	

I Minimal translationengleiche supergroups

[2]  $R\bar{3}m$  (166); [4]  $P\bar{4}3m$  (215); [4]  $F\bar{4}3m$  (216); [4]  $I\bar{4}3m$  (217)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

none

• Decreased unit cell

[3]  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$   $P31m$  (157)

## RHOMBOHEDRAL AXES

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

**General position**

Multiplicity,  
Wyckoff letter,  
Site symmetry

## Coordinates

6 c 1

(1)  $x, y, z$  (2)  $z, x, y$  (3)  $y, z, x$   
(4)  $z, y, x$  (5)  $y, x, z$  (6)  $x, z, y$

**I Maximal translationengleiche subgroups**

[2] $R31$ (146, $R3$ )	1; 2; 3	
{ [3] $R1m$ (8, $C1m1$ )	1; 4	$-a - c, -a + c, a + b + c$
	1; 5	$-a - b, a - b, a + b + c$
	1; 6	$-b - c, b - c, a + b + c$

**II Maximal klassengleiche subgroups**• **Loss of centring translations**

none

• **Enlarged unit cell**

[2] $\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{b} + \mathbf{c}$ $R3m$ (160)	$\langle 2; 4 \rangle$	$\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}$
[2] $\mathbf{a}' = \mathbf{a} + \mathbf{b}, \mathbf{b}' = \mathbf{b} + \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{c}$ $R3c$ (161)	$\langle 2; 4 + (1, 1, 1) \rangle$	$\mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{c}$
[3] $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$ $P3m1$ (156)	$\langle 2; 4 \rangle$	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$
[4] $\mathbf{a}' = \mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{b} - \mathbf{c}, \mathbf{c}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}$ $R3m$ (160)	$\langle 2; 4 \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$
$R3m$ (160)	$\langle 2 + (1, -2, 1); 4 + (1, 0, -1) \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$ 1, -1, 0
$R3m$ (160)	$\langle 2 + (1, 1, -2); 4 + (1, 0, -1) \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$ 0, 1, -1
$R3m$ (160)	$\langle 2 + (2, -1, -1); 4 + (2, 0, -2) \rangle$	$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$ 1, 0, -1

• **Series of maximal isomorphic subgroups**

[ $p$ ] $\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} + (p-2)\mathbf{b} + (p+1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p+1)\mathbf{a} + (p+1)\mathbf{b} + (p-2)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((p-2)\mathbf{a} + (p+1)\mathbf{b} + (p+1)\mathbf{c})$ $R3m$ (160)	$\langle 2; 4 \rangle$ $p > 1; p \equiv 2 \pmod{3}$ no conjugate subgroups	$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations})$
[ $p$ ] $\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} + (p-1)\mathbf{b} + (p-1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p-1)\mathbf{a} + (p+2)\mathbf{b} + (p-1)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((p-1)\mathbf{a} + (p-1)\mathbf{b} + (p+2)\mathbf{c})$ $R3m$ (160)	$\langle 2; 4 \rangle$ $p > 6; p \equiv 1 \pmod{3}$ no conjugate subgroups	$\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} \dots, \text{see lattice relations})$
[ $p^2$ ] $\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} + (1-2p)\mathbf{b} + (p+1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p+1)\mathbf{a} + (p+1)\mathbf{b} + (1-2p)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((1-2p)\mathbf{a} + (p+1)\mathbf{b} + (p+1)\mathbf{c})$ $R3m$ (160)	$\langle 2 + (u+v, -2u+v, u-2v); 4 + (u+v, 0, -u-v) \rangle$ $p > 1; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for prime $p \equiv 2 \pmod{3}$	$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations})$ $u, -u+v, -v$
[ $p^2$ ] $\mathbf{a}' = \frac{1}{3}((2p+1)\mathbf{a} + (1-p)\mathbf{b} + (1-p)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((1-p)\mathbf{a} + (2p+1)\mathbf{b} + (1-p)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((1-p)\mathbf{a} + (1-p)\mathbf{b} + (2p+1)\mathbf{c})$ $R3m$ (160)	$\langle 2 + (u+v, -2u+v, u-2v); 4 + (u+v, 0, -u-v) \rangle$ $p > 6; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for prime $p \equiv 1 \pmod{3}$	$\mathbf{a}' = \frac{1}{3}((2p+1)\mathbf{a} \dots, \text{see lattice relations})$ $u, -u+v, -v$

**I Minimal translationengleiche supergroups**

[2]  $R\bar{3}m$  (166); [4]  $P\bar{4}3m$  (215); [4]  $F\bar{4}3m$  (216); [4]  $I\bar{4}3m$  (217)

**II Minimal non-isomorphic klassengleiche supergroups**• **Additional centring translations**

none

• **Decreased unit cell**

[3]  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$   $P31m$  (157)