

$D_{3d}^6$ 
 $R\bar{3}2/c$ 

No. 167

 $R\bar{3}c$ 

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	<i>f</i>	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] $R\bar{3}c$ (161)	1; 2; 3; 10; 11; 12	
[2] $R\bar{3}2$ (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

[ $p$ ] $\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} + (p-2)\mathbf{b} + (p+1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p+1)\mathbf{a} + (p+1)\mathbf{b} + (p-2)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((p-2)\mathbf{a} + (p+1)\mathbf{b} + (p+1)\mathbf{c})$		
$R\bar{3}c$ (167)	$\langle 2; 4 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2u); 7 + (2u, 2u, 2u) \rangle$ $p > 4; 0 \leq u < p$ $p$ conjugate subgroups for prime $p \equiv 5 \pmod{6}$	$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations } u, u, u$
[ $p$ ] $\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} + (p-1)\mathbf{b} + (p-1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p-1)\mathbf{a} + (p+2)\mathbf{b} + (p-1)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((p-1)\mathbf{a} + (p-1)\mathbf{b} + (p+2)\mathbf{c})$		
$R\bar{3}c$ (167)	$\langle 2; 4 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2u); 7 + (2u, 2u, 2u) \rangle$ $p > 6; 0 \leq u < p$ $p$ conjugate subgroups for prime $p \equiv 1 \pmod{6}$	$\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} \dots, \text{see lattice relations } u, u, u$
[ $p^2$ ] $\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} + (1-2p)\mathbf{b} + (p+1)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((p+1)\mathbf{a} + (p+1)\mathbf{b} + (1-2p)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((1-2p)\mathbf{a} + (p+1)\mathbf{b} + (p+1)\mathbf{c})$		
$R\bar{3}c$ (167)	$\langle 2 + (u+v, -2u+v, u-2v); 4 + (u-v, -2u+2v, u-v); 7 + (2u, -2u+2v, -2v) \rangle$ $p > 1; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for prime $p \equiv 2 \pmod{3}$	$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations } u, -u+v, -v$
[ $p^2$ ] $\mathbf{a}' = \frac{1}{3}((2p+1)\mathbf{a} + (1-p)\mathbf{b} + (1-p)\mathbf{c}), \mathbf{b}' = \frac{1}{3}((1-p)\mathbf{a} + (2p+1)\mathbf{b} + (1-p)\mathbf{c}), \mathbf{c}' = \frac{1}{3}((1-p)\mathbf{a} + (1-p)\mathbf{b} + (2p+1)\mathbf{c})$		
$R\bar{3}c$ (167)	$\langle 2 + (u+v, -2u+v, u-2v); 4 + (u-v, -2u+2v, u-v); 7 + (2u, -2u+2v, -2v) \rangle$ $p > 6; p \equiv 1 \pmod{3}; 0 \leq u < p; 0 \leq v < p$ $p^2$ 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**

[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)