

$R3c$

No. 161

$R3c$

$C_{3v}^6$

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)

**General position**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

|    |                                     |  |  |
|----|-------------------------------------|--|--|
|    | (0,0,0)+                            | $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ | $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ |
| 18 | $b$                                 | 1  |  |
|    | (1) $x,y,z$                         | (2) $\bar{y},x-y,z$                      | (3) $\bar{x}+y,\bar{x},z$                |
|    | (4) $\bar{y},\bar{x},z+\frac{1}{2}$ | (5) $\bar{x}+y,y,z+\frac{1}{2}$          | (6) $x,x-y,z+\frac{1}{2}$                |

**I Maximal translationengleiche subgroups**

|                          |                             |   |
|--------------------------|-----------------------------|---|
| [2] $R31$ (146, $R3$ )   | $\langle 1; 2; 3 \rangle +$ |   |
| { [3] $R1c$ (9, $C1c1$ ) | $\langle 1; 4 \rangle +$    | $1/3(-\mathbf{a} + \mathbf{b} - 2\mathbf{c}), -\mathbf{a} - \mathbf{b}, \mathbf{c}$ |
| [3] $R1c$ (9, $C1c1$ )   | $\langle 1; 5 \rangle +$    | $1/3(-\mathbf{a} - 2\mathbf{b} - 2\mathbf{c}), \mathbf{a}, \mathbf{c}$              |
| [3] $R1c$ (9, $C1c1$ )   | $\langle 1; 6 \rangle +$    | $1/3(2\mathbf{a} + \mathbf{b} - 2\mathbf{c}), \mathbf{b}, \mathbf{c}$               |

**II Maximal klassengleiche subgroups**

• **Loss of centring translations**

[3]  $P3c1$  (158)                      1; 2; 3; 4; 5; 6

• **Enlarged unit cell**

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

|             |   |   |         |
|-------------|---|---|---------|
| $R3c$ (161) | $\langle 2; 4 \rangle$                          | $-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ |         |
| $R3c$ (161) | $\langle 2 + (1, -1, 0); 4 + (1, 1, 0) \rangle$ | $-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ | 1, 0, 0 |
| $R3c$ (161) | $\langle 2 + (1, 2, 0); 4 + (1, 1, 0) \rangle$  | $-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ | 0, 1, 0 |
| $R3c$ (161) | $\langle 2 + (2, 1, 0); 4 + (2, 2, 0) \rangle$  | $-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$ | 1, 1, 0 |

• **Series of maximal isomorphic subgroups**

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

|             |  |   |  |
|-------------|--|---|--|
| $R3c$ (161) | $\langle 2; 4 + (0, 0, \frac{p}{2} - \frac{1}{2}) \rangle$<br>$p > 4; p \equiv 5 \pmod{6}$<br>no conjugate subgroups | $-\mathbf{b}, \mathbf{a} + \mathbf{b}, p\mathbf{c}$ |  |
| $R3c$ (161) | $\langle 2; 4 + (0, 0, \frac{p}{2} - \frac{1}{2}) \rangle$<br>$p > 6; p \equiv 1 \pmod{6}$<br>no conjugate subgroups | $\mathbf{a}, \mathbf{b}, p\mathbf{c}$               |  |

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

|             |  |   |           |
|-------------|--|---|-----------|
| $R3c$ (161) | $\langle 2 + (u + v, -u + 2v, 0); 4 + (u + v, u + v, 0) \rangle$<br>$p > 1; 0 \leq u < p; 0 \leq v < p$<br>$p^2$ conjugate subgroups for prime $p \equiv 2 \pmod{3}$ | $-p\mathbf{b}, p\mathbf{a} + p\mathbf{b}, \mathbf{c}$ | $u, v, 0$ |
|-------------|--|---|-----------|

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

|             |  |  |           |
|-------------|--|--|-----------|
| $R3c$ (161) | $\langle 2 + (u + v, -u + 2v, 0); 4 + (u + v, u + v, 0) \rangle$<br>$p > 6; 0 \leq u < p; 0 \leq v < p$<br>$p^2$ conjugate subgroups for prime $p \equiv 1 \pmod{3}$ | $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ | $u, v, 0$ |
|-------------|--|--|-----------|

**I Minimal translationengleiche supergroups**

[2]  $R\bar{3}c$  (167); [4]  $P\bar{4}3n$  (218); [4]  $F\bar{4}3c$  (219); [4]  $I\bar{4}3d$  (220)

**II Minimal non-isomorphic klassengleiche supergroups**

• **Additional centring translations**

none

• **Decreased unit cell**

[3]  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$   $P31c$  (159); [2]  $\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$   $R3m$  (160)

## 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 | <i>b</i> | 1 | (1) $x, y, z$   | (2) $z, x, y$   | (3) $y, z, x$   |
|   |          |   | (4) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ | (5) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ | (6) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ |

I Maximal *translationengleiche* subgroups

|                   |         |  |
|-------------------|---------|--|
| [2] R31 (146, R3) | 1; 2; 3 |  |
| [3] R1c (9, C1c1) | 1; 4    | $-\mathbf{a} - \mathbf{c}, -\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$ |
| [3] R1c (9, C1c1) | 1; 5    | $-\mathbf{a} - \mathbf{b}, \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b} + \mathbf{c}$  |
| [3] R1c (9, C1c1) | 1; 6    | $-\mathbf{b} - \mathbf{c}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$  |

II Maximal *klassengleiche* subgroups

## • Loss of centring translations

none

## • Enlarged unit cell

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

P3c1 (158) (2; 4)

$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$

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

R3c (161) (2; 4)  
 R3c (161)  $\langle 2 + (1, -2, 1); 4 + (1, 0, -1) \rangle$   
 R3c (161)  $\langle 2 + (1, 1, -2); 4 + (1, 0, -1) \rangle$   
 R3c (161)  $\langle 2 + (2, -1, -1); 4 + (2, 0, -2) \rangle$

$\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$   
 $\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$  1, -1, 0  
 $\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$  0, 1, -1  
 $\mathbf{a} - \mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{b} - \mathbf{c}, -\mathbf{a} + \mathbf{b} + \mathbf{c}$  1, 0, -1

## • Series of maximal isomorphic subgroups

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

R3c (161)  $\langle 2; 4 + (\frac{p}{2} - \frac{1}{2}, \frac{p}{2} - \frac{1}{2}, \frac{p}{2} - \frac{1}{2}) \rangle$   
 $p > 4; p \equiv 5 \pmod{6}$

$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations})$

no conjugate subgroups

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

R3c (161)  $\langle 2; 4 + (\frac{p}{2} - \frac{1}{2}, \frac{p}{2} - \frac{1}{2}, \frac{p}{2} - \frac{1}{2}) \rangle$   
 $p > 6; p \equiv 1 \pmod{6}$

$\mathbf{a}' = \frac{1}{3}((p+2)\mathbf{a} \dots, \text{see lattice relations})$

no conjugate subgroups

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

R3c (161)  $\langle 2 + (u+v, -2u+v, u-2v); 4 + (u+v, 0, -u-v) \rangle$   
 $p > 1; 0 \leq u < p; 0 \leq v < p$

$\mathbf{a}' = \frac{1}{3}((p+1)\mathbf{a} \dots, \text{see lattice relations})$   
 $u, -u+v, -v$

$p^2$  conjugate subgroups for prime  $p \equiv 2 \pmod{3}$

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

R3c (161)  $\langle 2 + (u+v, -2u+v, u-2v); 4 + (u+v, 0, -u-v) \rangle$   
 $p > 6; 0 \leq u < p; 0 \leq v < p$

$\mathbf{a}' = \frac{1}{3}((2p+1)\mathbf{a} \dots, \text{see lattice relations})$   
 $u, -u+v, -v$

$p^2$  conjugate subgroups for prime  $p \equiv 1 \pmod{3}$

I Minimal *translationengleiche* supergroups

[2]  $R\bar{3}c$  (167); [4]  $P\bar{4}3n$  (218); [4]  $F\bar{4}3c$  (219); [4]  $I\bar{4}3d$  (220)

II Minimal non-isomorphic *klassengleiche* supergroups

## • Additional centring translations

none

## • Decreased unit cell

[3]  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$  P31c (159);

[2]  $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}), \mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}), \mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$  R3m (160)