

$C_3^4$ 
 $R3$ 

No. 146

 $R3$ 

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)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

	$(0,0,0)+$	$(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})+$	$(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})+$
9	$b$	1	
	(1) $x,y,z$	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$

**I Maximal translationengleiche subgroups**

[3] $R1$ (1, $P1$ )	1+	$\mathbf{a}, \mathbf{b}, 1/3(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$
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**II Maximal klassengleiche subgroups**

## • Loss of centring translations

[3] $P3_2$ (145)	1; $2 + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$ ; $3 + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$	0, 1/3, 0
[3] $P3_1$ (144)	1; $2 + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ ; $3 + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$	1/3, 1/3, 0
[3] $P3$ (143)	1; 2; 3	

## • Enlarged unit cell

[2] $\mathbf{a}' = -\mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
$R3$ (146)	$\langle 2 \rangle$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$
[4] $\mathbf{a}' = -2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$		
$R3$ (146)	$\langle 2 \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
$R3$ (146)	$\langle 2 + (1, -1, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
$R3$ (146)	$\langle 2 + (1, 2, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$
$R3$ (146)	$\langle 2 + (2, 1, 0) \rangle$	$-2\mathbf{b}, 2\mathbf{a} + 2\mathbf{b}, \mathbf{c}$

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$		
$R3$ (146)	$\langle 2 \rangle$	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, p\mathbf{c}$
	$p > 1; p \equiv 2 \pmod{3}$	
	no conjugate subgroups	
$R3$ (146)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$p > 6; p \equiv 1 \pmod{3}$	
	no conjugate subgroups	
[ $p^2$ ] $\mathbf{a}' = -p\mathbf{b}, \mathbf{b}' = p\mathbf{a} + p\mathbf{b}$		
$R3$ (146)	$\langle 2 + (u + v, -u + 2v, 0) \rangle$	$-p\mathbf{b}, p\mathbf{a} + p\mathbf{b}, \mathbf{c}$
	$p > 1; 0 \leq u < p; 0 \leq v < p$	$u, v, 0$
	$p^2$ conjugate subgroups for prime $p \equiv 2 \pmod{3}$	
[ $p = q^2 + r^2 - qr$ ] $\mathbf{a}' = (q - r)\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$		
$R3$ (146)	$\langle 2 + (u, -u, 0) \rangle$	$(q - r)\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$
	$q > 0; r > 0; q \neq r; q + r \equiv 1 \pmod{3}; p > 6;$	$u, 0, 0$
	$0 \leq u < p$	
	$p$ conjugate subgroups for each pair of $q$ and $r$	

**I Minimal translationengleiche supergroups**

 [2]  $R\bar{3}$  (148); [2]  $R32$  (155); [2]  $R3m$  (160); [2]  $R3c$  (161); [4]  $P23$  (195); [4]  $F23$  (196); [4]  $I23$  (197); [4]  $P2_13$  (198); [4]  $I2_13$  (199)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

none

## • Decreased unit cell

 [3]  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$   $P3$  (143)

RHOMBOHEDRAL AXES

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

General position

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

3 b 1

(1)  $x, y, z$  (2)  $z, x, y$  (3)  $y, z, x$

I Maximal *translationengleiche* subgroups

[3] R1 (1, P1) 1

II Maximal *klassengleiche* subgroups

• Loss of centring translations

none

• Enlarged unit cell

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

R3 (146)  $\langle 2 \rangle$

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

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

$P3_2$  (145)  $\langle 2 + (1, 1, 0) \rangle$

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

$0, 1/3, -1/3$

$P3_1$  (144)  $\langle 2 + (1, 0, 0) \rangle$

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

$1/3, 0, -1/3$

P3 (143)  $\langle 2 \rangle$

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

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

R3 (146)  $\langle 2 \rangle$

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

R3 (146)  $\langle 2 + (1, -2, 1) \rangle$

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

$1, -1, 0$

R3 (146)  $\langle 2 + (1, 1, -2) \rangle$

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

$0, 1, -1$

R3 (146)  $\langle 2 + (2, -1, -1) \rangle$

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

$1, 0, -1$

• Series of maximal isomorphic subgroups

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

R3 (146)  $\langle 2 \rangle$

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

$p > 1$ ;  $p \equiv 2 \pmod{3}$

no conjugate subgroups

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

R3 (146)  $\langle 2 \rangle$

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

$p > 6$ ;  $p \equiv 1 \pmod{3}$

no conjugate subgroups

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

R3 (146)  $\langle 2 + (u+v, -2u+v, u-2v) \rangle$

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

$p > 1$ ;  $0 \leq u < p$ ;  $0 \leq v < p$

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

$u, -u+v, -v$

[ $p = q^2 + r^2 - qr$ ]  $\mathbf{a}' = \frac{1}{3}(\alpha\mathbf{a} + \beta\mathbf{b} + \gamma\mathbf{c})$ ,  $\mathbf{b}' = \frac{1}{3}(\gamma\mathbf{a} + \alpha\mathbf{b} + \beta\mathbf{c})$ ,  $\mathbf{c}' = \frac{1}{3}(\beta\mathbf{a} + \gamma\mathbf{b} + \alpha\mathbf{c})$ ;  $\alpha = 2q - r + 1$ ,  $\beta = 1 - q - r$ ,  $\gamma = 2r + 1 - q$

R3 (146)  $\langle 2 + (u, -2u, u) \rangle$

$\mathbf{a}' = \frac{1}{3}(\alpha\mathbf{a} + \beta\mathbf{b} \dots$ , see lattice relations

$q > 0$ ;  $r > 0$ ;  $q \neq r$ ;  $q + r \equiv 1 \pmod{3}$ ;  $p > 6$ ;

$0 \leq u < p$

$u, -u, 0$

$p$  conjugate subgroups for each pair of  $q$  and  $r$

I Minimal *translationengleiche* supergroups

[2]  $R\bar{3}$  (148); [2] R32 (155); [2] R3m (160); [2] R3c (161); [4] P23 (195); [4] F23 (196); [4] I23 (197); [4] P2<sub>1</sub>3 (198); [4] I2<sub>1</sub>3 (199)

II Minimal non-isomorphic *klassengleiche* supergroups

• Additional centring translations

none

• Decreased unit cell

[3]  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ ,  $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ ,  $\mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$  P3 (143)