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+	$\mathbf{a},\mathbf{b},1/3(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	

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

- **Series of maximal isomorphic subgroups**

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

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)

$R3$ No. 146 $R3$ C_3^4

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

$R3$ (146) $\langle 2\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
p prime; $p=2$ or $p=6n-1$
no conjugate subgroups

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

$R3$ (146) $\langle 2\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations
prime $p=6n+1$
no conjugate subgroups

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

$R3$ (146) $\langle 2+(u+v,-2u+v,u-2v)\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
p prime; $0\le u<p$; $0\le v<p$ $u,-u+v,-v$
p^2 conjugate subgroups for $p=2$ or $p=6n-1$

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

$R3$ (146) $\langle 2+(u,-2u,u)\rangle$ $\mathbf{a}'=\frac{1}{3}(\alpha\mathbf{a}+\beta\mathbf{b}\ldots$, see lattice relations
prime $p=6n+1$; $q>0$; $r>0$; $q\neq r$; $u,-u,0$
$q+r=3n'+1$; $0\le u<p$
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] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\ \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\ \mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P3$ (143)