① # $R3$ No. 146 $R3$ C_3^4

HEXAGONAL AXES

② **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) $\bar{x}+y,\bar{x},z$

③ **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

④ • **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		

⑤ • **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)	$\langle 2+(2,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

⑥ • **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	$(q-r)\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

⑦ **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)

⑧ **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)

Data for the maximal subgroups $\mathcal{H}_i$ of the space group $\mathcal{G}$, here $R3$, are given in items ① to ⑥ and data for the minimal supergroups $\mathcal{G}_k$ of the space group $\mathcal{H}$, here $R3$, are given in items ⑦ and ⑧.

① *Headline*. From the outside margin inwards [taken from Volume A of *International Tables for Crystallography* (*IT* A); for explanations, *cf.* Section 2.1.2.1]:

Short Hermann–Mauguin symbol	Number of space group according to Volume A	Full Hermann–Mauguin symbol	Schoenflies symbol

An additional line for monoclinic and rhombohedral space groups specifies the cell setting, here hexagonal axes; for space groups with origin choice 1 and 2 it specifies the origin, *cf.* Sections 2.1.2.3 and 2.1.2.5.

② *Generators selected*: complete set of generators of the space group $\mathcal{G}$, taken from *IT* A, *cf.* Section 2.1.2.2.

General position of $\mathcal{G}$, taken from the first entry under *Positions* of $\mathcal{G}$ in *IT* A, *cf.* Section 2.1.2.2.

③ List of all *Maximal translationengleiche subgroups* of $\mathcal{G}$, *cf.* Section 2.1.3. Listed from left to right are: index (in square brackets); space-group specification; general position of $\mathcal{H}$ referred to the general position of $\mathcal{G}$; basis transformation; origin shift. Conjugacy classes of subgroups are connected by left braces.

The *Maximal klassengleiche subgroups* $\mathcal{H}$ of the space group $\mathcal{G}$ are separated into three blocks, *cf.* Section 2.1.4.1. Each block is marked by a bullet, •.

④ *Loss of centring translations*: List of all maximal *klassengleiche* subgroups of index 2, 3 and 4 which have fully or partly lost their conventional lattice centrings, *cf.* Section 2.1.4.2. This block is omitted for space groups with the lattice symbol *P* in the Hermann–Mauguin (HM) symbol. Listed from left to right are: index (in square brackets); space-group specification; general position of $\mathcal{H}$ referred to the general position of $\mathcal{G}$; basis transformation; origin shift. Conjugacy classes of subgroups are connected by left braces.

⑤ *Enlarged unit cell*. List of all maximal *klassengleiche* subgroups $\mathcal{H}$ of index 2, 3 and 4 whose conventional unit cell is larger than that of $\mathcal{G}$, *cf.* Section 2.1.4.3. Listed from left to right are: index (in square brackets); basis vectors $\mathbf{a}_i'$ of the lattice of $\mathcal{H}$ expressed in the basis $(\mathbf{a}_k)^{\mathrm{T}}$ of $\mathcal{G}$ (if $\mathbf{a}_i' \neq \mathbf{a}_i$); (on a new line:) space-group specification; set of generators of $\mathcal{H}$ referred to the general position of $\mathcal{G}$; basis transformation; origin shift. Conjugacy classes of subgroups are connected by braces.

⑥ *Series of maximal isomorphic subgroups*, *cf.* Section 2.1.5. Listed from left to right are: index of $\mathcal{H}$ (in square brackets; p is prime, q and r are integers); basis vectors $\mathbf{a}_i'$ of the lattice of $\mathcal{H}$ expressed in the basis $(\mathbf{a}_k)^{\mathrm{T}}$ of $\mathcal{G}$ (if $\mathbf{a}_i' \neq \mathbf{a}_i$); (on a new line:) space-group specification; set of generators of $\mathcal{H}$ referred to the general position of $\mathcal{G}$; basis transformation; origin shift; (on a new line:) description of the conjugacy classes.

⑦ *Minimal translationengleiche supergroups* $\mathcal{G}$ of the space group $\mathcal{H}$ (here $R3$), *cf.* Section 2.1.6.2. Listed from left to right are: index of $\mathcal{G}$ (in square brackets); conventional HM symbol of $\mathcal{G}$; space-group number of $\mathcal{G}$ (in parentheses).

⑧ The *Minimal non-isomorphic klassengleiche supergroups* are divided into two blocks, *cf.* Section 2.1.6.3. Each block is marked by a bullet, •.

Additional centring translations. Listed are: index of $\mathcal{G}$ (in square brackets); space-group specification.

Decreased unit cell. Listed are: index of $\mathcal{G}$ (in square brackets); basis vectors $\mathbf{a}_i'$ of the lattice of $\mathcal{G}$ expressed in the basis $(\mathbf{a}_k)^{\mathrm{T}}$ of $\mathcal{H}$ (if $\mathbf{a}_i' \neq \mathbf{a}_i$); space-group specification.

① *Aem*2 — No. 39 — no full symbol in this case — C_{2v}^{15}

②	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	4*c*	8*d*
③ **I Maximal *translationengleiche* subgroups**						
[2] *A*1*m*1 (8)		$x,y+\frac{1}{4},z$	4*b*	4*b*	2×2*a*	2×4*b*
$\widehat{=}$ *C*1*m*1	**c**, −**b**, **a**	$z,-y-\frac{1}{4},x$				
[2] *Pb*11 (7)	**a**, **b**, $\frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x,y+z,2z$	2*a*	2*a*	2*a*	2×2*a*
$\widehat{=}$ *P*1*c*1	$\frac{1}{2}(-\mathbf{b}+\mathbf{c})$, **a**, **b**	$2z,x,y+z$				
[2] *A*112 (5)			2×2*a*	2×2*b*	4*c*	2×4*c*
④ **II Maximal *klassengleiche* subgroups**						
Loss of centring translations						
[2] *Pbc*2_1 (29)		$x,y+\frac{1}{4},z$	4*a*	4*a*	4*a*	2×4*a*
$\widehat{=}$ *Pca*2_1	**b**, −**a**, **c**	$y+\frac{1}{4},-x,z$				
[2] *Pbm*2 (28)			2×2*a*	2×2*b*	2×2*c*	2×4*d*
$\widehat{=}$ *Pma*2	**b**, −**a**, **c**	$y,-x,z$				
[2] *Pcc*2 (27)			2*a*; 2*b*	2*c*; 2*d*	4*e*	2×4*e*
[2] *Pcm*2_1 (26)		$x,y+\frac{1}{4},z$	4*c*	4*c*	2*a*; 2*b*	2×4*c*
$\widehat{=}$ *Pmc*2_1	**b**, −**a**, **c**	$y+\frac{1}{4},-x,z$				
Enlarged unit cell, non-isomorphic						
[2] *Ibm*2 (46)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	2×4*a*	8*c*	2×4*b*	2×8*c*
$\widehat{=}$ *Ima*2	**b**, 2**a**, −**c**	$y,\frac{1}{2}x,-z;\ +(0,\frac{1}{2},0)$				
[2] *Ibm*2 (46)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	8*c*	2×4*a*	2×4*b*	2×8*c*
$\widehat{=}$ *Ima*2	**b**, 2**a**, −**c**	$y,\frac{1}{2}x+\frac{1}{4},-z;\ +(0,\frac{1}{2},0)$				
[2] *Iba*2 (45)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	4*a*; 4*b*	8*c*	8*c*	2×8*c*
[2] *Iba*2 (45)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	8*c*	4*a*; 4*b*	8*c*	2×8*c*
[2] *Aea*2 (41)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	2×4*a*	8*b*	8*b*	2×8*b*
[2] *Aea*2 (41)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	8*b*	2×4*a*	8*b*	2×8*b*
Enlarged unit cell, isomorphic						
[2] *Aem*2	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	4*a*; 4*b*	8*d*	2×4*c*	2×8*d*
[2] *Aem*2	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	8*d*	4*a*; 4*b*	2×4*c*	2×8*d*
[3] *Aem*2	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	4*a*; 8*d*	4*b*; 8*d*	3×4*c*	3×8*d*
[*p*] *Aem*2	*p***a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	4*a*; $\frac{p-1}{2}$×8*d*	4*b*; $\frac{p-1}{2}$×8*d*	*p*×4*c*	*p*×8*d*
	p = prime > 2; $u = 1,\dots,p-1$					
[3] *Aem*2	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	4*a*; 8*d*	4*b*; 8*d*	4*c*; 8*d*	3×8*d*
[*p*] *Aem*2	**a**, *p***b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	4*a*; $\frac{p-1}{2}$×8*d*	4*b*; $\frac{p-1}{2}$×8*d*	4*c*; $\frac{p-1}{2}$×8*d*	*p*×8*d*
	p = prime > 2; $u = 1,\dots,p-1$					
[3] *Aem*2	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	3×4*a*	3×4*b*	3×4*c*	3×8*d*
[*p*] *Aem*2	**a**, **b**, *p***c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	*p*×4*a*	*p*×4*b*	*p*×4*c*	*p*×8*d*
	p = prime > 2; $u = 1,\dots,p-1$					

⑤ **Nonconventional settings**

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

*B*2*em*	$A \to B;\ C \to A$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
*Cm*2*e*	$A \to C;\ C \to B$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
*Bme*2	$A \to B$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
*C*2*me*	$A \rightleftarrows C$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
*Ae*2*m*	$C \to B$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

① *Headline*. From the outside margin inwards:

Short Hermann–Mauguin symbol	Number of space group according to Volume A	Full Hermann–Mauguin symbol (given only if it differs from the short symbol)	Schoenflies symbol

An additional line for monoclinic and rhombohedral space groups specifies the cell setting, *cf.* Section 3.1.1.2.

② Unit-cell transformations are given in the column 'Axes'	Coordinate transformations are given in the column 'Coordinates'	List of the Wyckoff positions of the space group

③ List of the *translationengleiche* subgroups and all of their Wyckoff positions:

Index (in square brackets);
Short Hermann–Mauguin symbol and space-group number of the subgroup;
Basis vectors in terms of the basis vectors of the space group, *cf.* Section 3.1.1.6.3 (given only if the cell settings of the space group and the subgroup differ);
Coordinates in the subgroup from the coordinates x, y, z of the space group, including origin shifts, *cf.* Section 3.1.1.6.4 (given only if the coordinates of the space group and the subgroup differ);
Wyckoff positions resulting from the Wyckoff positions of the space group, *cf.* Section 3.1.1.6.5.

If a nonconventional setting of the subgroup is listed first, the conventional setting and the corresponding cell and coordinate transformations are given after the symbol $\widehat{=}$. Sometimes several different settings for the same subgroup are listed after the word 'or'.

Note: Origin shifts are given as additive fractional numbers in the column 'Coordinates' and thus do not refer to the coordinate system of the space group, but to the coordinate systems of the subgroups. The values for an origin shift referred to the coordinate system of the space group can be obtained by the transformation described in Section 3.1.3. The origin shifts given in Part 3 are usually different from the origin shifts in Part 2 of this volume.

④ List of the *klassengleiche* subgroups and all of their Wyckoff positions, listed in the same manner as for the *translationengleiche* subgroups. This is divided into three blocks:

Loss of centring translations;
Non-isomorphic subgroups with enlarged unit cell;
Isomorphic subgroups with enlarged unit cell.

If there are no subgroups in one of these blocks, the block is omitted.
An index value p may be any prime number according to the given limits.

⑤ For orthorhombic space groups only: list of nonconventional settings of the space group. If a nonconventional setting is used, the sequence of the symbols and the symbols themselves have to be interchanged as specified for *all* entries of *every* subgroup in its Hermann–Mauguin symbol, its basis vectors and its coordinates, *cf.* Section 3.1.4.

An entry such as $A \to B$; $C \to A$ and $a \to b \to c \to a$ means: convert A to B, convert C to A, convert a to b, convert b to c, convert c to a; simultaneously exchange the positions in the Hermann–Mauguin symbol of all subgroups. Thus, the following subgroup symbols have to be replaced as shown:

$A1m1 \to B11m$	$Pbc2_1 \to P2_1ca$	$Ibm2 \to I2cm$
$Pb11 \to P1c1$	$Pbm2 \to P2cm$	$Iba2 \to I2cb$
$A112 \to B211$	$Pcc2 \to P2aa$	$Aea2 \to B2eb$

If in the column 'Axes' the entry for a subgroup reads '$2\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$' and the interconversion is given as '$\mathbf{a} \rightleftarrows -\mathbf{b}$', then for the nonconventional setting the axes transformation is $\mathbf{a}$, $-2\mathbf{b}$, $\mathbf{c}$, *i.e.* $2\mathbf{a}$ and $\mathbf{b}$ change places and labels. Correspondingly, for the interconversion '$x \rightleftarrows -y$' the entry '$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2},0,0)$' in the column 'Coordinates' has to be converted to '$x, -\frac{1}{2}y-\frac{1}{4}, z; +(0,-\frac{1}{2},0)$'.