International Tables for Crystallography (2006). Vol. A1, Section 2.1.3, pp. 45–48.

On the other hand, the origin is situated on an inversion centre for origin choice 2 of $\mathcal{G}(2)$, as is the origin in the conventional description of the three monoclinic maximal *t*-subgroups. For them the origin shift is $\boldsymbol{p}_2 = \boldsymbol{o}$, while there is a nonzero column $\boldsymbol{p}_2$ for the orthorhombic subgroups.

(*b*) Both $\mathcal{G}$ and its subgroup $\mathcal{H} < \mathcal{G}$ are listed with two origins. Then the origin choice of $\mathcal{H}$ is the same as that of $\mathcal{G}$. This rule always applies to isomorphic subgroups as well as in some other cases.

Example 2.1.2.5.5.

Maximal *k*-subgroups $\mathcal{H}$: *Pnnn*, No. 48, of the space group $\mathcal{G}$: *Pban*, No. 50. There are two such subgroups with the lattice relation $\mathbf{c}' = 2\mathbf{c}$. Both $\mathcal{G}$ and $\mathcal{H}$ are listed with two origins such that the origin choices of $\mathcal{G}$ and $\mathcal{H}$ are either the same or are strongly related.

(*c*) The group $\mathcal{G}$ is listed with one origin but the subgroup $\mathcal{H} < \mathcal{G}$ is listed with two origins. This situation is restricted to maximal *k*-subgroups with the only exception being $Ia\bar{3}d > I4_1/acd$, where there are three conjugate *t*-subgroups of index 3. In all cases the subgroup $\mathcal{H}$ is referred to origin choice 2. This rule is followed in the subgroup tables because it gives a better chance of retaining the origin of $\mathcal{G}$ in $\mathcal{H}$. If there are two origin choices for $\mathcal{H}$, then $\mathcal{H}$ has inversions and these are also elements of the supergroup $\mathcal{G}$. The (unique) origin of $\mathcal{G}$ is placed on one of the inversion centres. For origin choice 2 in $\mathcal{H}$, the origin of $\mathcal{H}$ may agree with that of $\mathcal{G}$, although this is not guaranteed. In addition, origin choice 2 is often preferred in structure determinations.

Example 2.1.2.5.6.

Maximal *k*-subgroups of *Pccm*, No. 49. In the block

• **Enlarged unit cell**, [2] $\mathbf{a}' = 2\mathbf{a}$

one finds two subgroups *Pcna* (50, *Pban*). One of them has the origin of $\mathcal{G}$, the origin of the other subgroup is shifted by $\frac{1}{2}, 0, 0$ and is placed on one of the inversion centres of $\mathcal{G}$ that is removed from the first subgroup. The analogous situation is found in the block [2] $\mathbf{b}' = 2\mathbf{b}$, where the two subgroups of space-group type *Pncb* (50, *Pban*) show the analogous relation. In the next block, [2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, the four subgroups *Ccce* (68) behave similarly.

For $\mathcal{G}$ = *Pmma*, No. 51, the same holds for the two subgroups of the type *Pmmn* (59) in the block [2] $\mathbf{b}' = 2\mathbf{b}$.

On the other hand, for $\mathcal{G}$ = *Immm*, No. 71, in the block 'Loss of centring translations' three subgroups of type *Pmmn* (59) and one of type *Pnnn* (48) are listed. All of them need an origin shift of $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ because they have lost the inversion centres of the origin of $\mathcal{G}$.

2.1.2.5.3. *Space groups with a rhombohedral lattice*

The seven trigonal space groups with a rhombohedral lattice are often called *rhombohedral space groups*. Their HM symbols begin with the lattice letter *R* and they are listed with both hexagonal axes and rhombohedral axes.

Rules:

(*a*) A rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is listed in the same setting as $\mathcal{G}$: if $\mathcal{G}$ is referred to hexagonal axes, so is $\mathcal{H}$; if $\mathcal{G}$ is referred to rhombohedral axes, so is $\mathcal{H}$.

(*b*) If $\mathcal{G}$ is a non-rhombohedral trigonal or a cubic space group, then a rhombohedral subgroup $\mathcal{H} < \mathcal{G}$ is always referred to hexagonal axes.

(*c*) A non-rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is referred to its standard setting.

Remarks:

Rule (*a*) provides a clear definition, in particular for the axes of isomorphic subgroups.

Rule (*b*) has been followed in the subgroup tables because the rhombohedral setting is rarely used in crystallography.

Rule (*c*) implies that monoclinic subgroups of rhombohedral space groups are referred to the setting 'unique axis *b*'.

There is a peculiarity caused by the two settings. The rhombohedral lattice appears to be centred in the hexagonal axes setting, whereas it is primitive in the rhombohedral axes setting. Therefore, there are trigonal subgroups of a rhombohedral space group $\mathcal{G}$ which are listed in the block 'Loss of centring translations' for the hexagonal axes setting of $\mathcal{G}$ but are listed in the block 'Enlarged unit cell' when $\mathcal{G}$ is referred to rhombohedral axes. Although unnecessary and not done for other space groups with primitive lattices, the line

• **Loss of centring translations** none

is listed for the rhombohedral axes setting.

Example 2.1.2.5.7.

$\mathcal{G} = R3$, No. 146. Maximal *klassengleiche* subgroups of index 2 and 3. Comparison of the subgroup data for the two settings of *R*3 shows that the subgroups $P3_2$ (145), $P3_1$ (144) and *P*3 (143) of index 3 appear in the block 'Loss of centring translations' for the hexagonal setting and in the block 'Enlarged unit cell' for the rhombohedral setting.

The sequence of the blocks has priority over the classification by increasing index. Therefore, in the setting 'hexagonal axes', the subgroups of index 3 precede the subgroup of index 2.

The complete general position is listed for the maximal *k*-subgroups of index 3 in the setting 'hexagonal axes'; only the generator is listed for rhombohedral axes.

2.1.3. I Maximal *translationengleiche* subgroups (*t*-subgroups)

2.1.3.1. *Introduction*

In this block, all maximal *t*-subgroups $\mathcal{H}$ of the plane groups and the space groups $\mathcal{G}$ are listed individually. Maximal *t*-subgroups are always non-isomorphic.

For the sequence of the subgroups, see Section 2.1.2.4. There are no lattice relations for *t*-subgroups because the lattice is retained. Therefore, the sequence is determined only by the rising value of the index and by the decreasing space-group number.

2.1.3.2. *A description in close analogy with IT A*

The listing is similar to that of *IT* A and presents on one line the following information for each subgroup $\mathcal{H}$:

[*i*] HMS1 (No., HMS2) sequence matrix shift

Conjugate subgroups are listed together and are connected by a left brace.

The symbols have the following meaning:

[i]	index of $\mathcal{H}$ in $\mathcal{G}$;
HMS1	HM symbol of $\mathcal{H}$ referred to the coordinate system and setting of $\mathcal{G}$. This symbol may be nonconventional;
No.	space-group No. of $\mathcal{H}$;
HMS2	conventional HM symbol of $\mathcal{H}$ if HMS1 is not a conventional HM symbol;
sequence	sequence of numbers; the numbers refer to those coordinate triplets of the general position of $\mathcal{G}$ that are retained in $\mathcal{H}$, *cf. Remarks*; for general position *cf.* Section 2.1.2.2.2;
matrix	matrix part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3;
shift	column part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3.

Remarks:

In the sequence column for space groups with centred lattices, the abbreviation '(numbers)+' means that the coordinate triplets specified by 'numbers' are to be taken plus those obtained by adding each of the centring translations, see the comments following Examples 2.1.3.2.1 and 2.1.3.2.2.

The symbol HMS2 is omitted if HMS1 is a conventional HM symbol.

The following deviations from the listing of *IT* A are introduced in these tables:

No.: the space-group No. of $\mathcal{H}$ is added.

HMS2: In order to specify the setting clearly, the *full* HM symbol is listed for monoclinic subgroups, not the standard (short) HM symbol as in *IT* A.

matrix, shift: These entries contain information on the transformation of $\mathcal{H}$ from the setting of $\mathcal{G}$ to the standard setting of $\mathcal{H}$. They are explained in Section 2.1.3.3.

The description of the subgroups can be explained by the following four examples.

Example 2.1.3.2.1.
$\mathcal{G}$: $C1m1$, No. 8, UNIQUE AXIS b

I Maximal *translationengleiche* subgroups

[2] $C1$ (1, $P1$) 1+

Comments:

HMS1: $C1$ is not a conventional HM symbol. Therefore, the conventional symbol $P1$ is added as HMS2 after the space-group number 1 of $\mathcal{H}$.

sequence: '1+' means x, y, z; $x+\frac{1}{2}, y+\frac{1}{2}, z$.

Example 2.1.3.2.2.
$\mathcal{G}$: $Fdd2$, No. 43

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...

[2] $F112$ (5, $A112$) (1; 2)+

Comments:

HMS1: $F112$ is not a conventional HM symbol; therefore, the conventional symbol $A112$ is added to the space-group No. 5 as HMS2. The setting unique axis c is inherited from $\mathcal{G}$.

sequence: (1, 2)+ means:
x, y, z; $x, y+\frac{1}{2}, z+\frac{1}{2}$; $x+\frac{1}{2}, y, z+\frac{1}{2}$; $x+\frac{1}{2}, y+\frac{1}{2}, z$;
$\bar{x}, \bar{y}, z$; $\bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$; $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$; $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$;

Example 2.1.3.2.3.
$\mathcal{G}$: $P4_2/nmc = P4_2/n\,2_1/m\,2/c$, No. 137, ORIGIN CHOICE 2

I Maximal *translationengleiche* subgroups

...

[2] $P2/n\,2_1/m\,1$ (59, $Pmmn$) 1; 2; 5; 6; 9; 10; 13; 14

Comments:

HMS1: The sequence in the HM symbol for a tetragonal space group is **c**, **a**, **a** − **b**. From the parts $4_2/n$, $2_1/m$ and $2/c$ of the full HM symbol of $\mathcal{G}$, only $2/n$, $2_1/m$ and 1 remain in $\mathcal{H}$. Therefore, HMS1 is $P2/n\,2_1/m\,1$, and the conventional symbol $Pmmn$ is added as HMS2.

No.: The space-group number of $\mathcal{H}$ is 59. The setting origin choice 2 of $\mathcal{H}$ is inherited from $\mathcal{G}$.

sequence: The coordinate triplets of $\mathcal{G}$ retained in $\mathcal{H}$ are: (1) x, y, z; (2) $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$; (5) $\bar{x}, y+\frac{1}{2}, \bar{z}$; (6) $x+\frac{1}{2}, \bar{y}, \bar{z}$; (9) $\bar{x}, \bar{y}, \bar{z}$; *etc.*

Example 2.1.3.2.4.
$\mathcal{G}$: $P3_112$, No. 151

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[2] $P3_111$ (144, $P3_1$)	1; 2; 3		
{ [3] $P112$ (5, $C121$)	1; 6	**b**, −2**a**−**b**, **c**	
[3] $P112$ (5, $C121$)	1; 4	−**a**−**b**, **a**−**b**, **c**	0, 0, 1/3
[3] $P112$ (5, $C121$)	1; 5	**a**, **a**+2**b**, **c**	0, 0, 2/3

Comments:

brace: The brace on the left-hand side connects the three conjugate monoclinic subgroups.

HMS1: $P112$ is not the conventional HM symbol for unique axis c but the constituent '2' of the nonconventional HM symbol refers to the directions $-2\mathbf{a}-\mathbf{b}$, $\mathbf{a}-\mathbf{b}$ and $\mathbf{a}+2\mathbf{b}$, in the hexagonal basis. According to the rules of Section 2.1.2.5, the standard setting is unique axis b, as expressed by the HM symbol $C121$.

HMS2: Note that the conventional monoclinic cell is centred.

matrix, shift: The entries in the columns 'matrix' and 'shift' are explained in the following Section 2.1.3.3 and evaluated in Example 2.1.3.3.2.

2.1.3.3. *Basis transformation and origin shift*

Each t-subgroup $\mathcal{H} < \mathcal{G}$ is defined by its representatives, listed under 'sequence' by numbers each of which designates an element of $\mathcal{G}$. These elements form the general position of $\mathcal{H}$. They are taken from the general position of $\mathcal{G}$ and, therefore, are referred to the coordinate system of $\mathcal{G}$. In the general position of $\mathcal{H}$, however, its elements are referred to the coordinate system of $\mathcal{H}$. In order to allow the transfer of the data from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$, the tools for this transformation are provided in the columns 'matrix' and 'shift' of the subgroup tables. The designation of the quantities is that of *IT* A Part 5 and is repeated here for convenience.

In the following, columns and rows are designated by boldface italic lower-case letters. Point coordinates $\boldsymbol{x}, \boldsymbol{x}'$, translation parts $\boldsymbol{w}$, $\boldsymbol{w}'$ of the symmetry operations and shifts $\boldsymbol{p}$, $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$ are represented by columns. The sets of basis vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\boldsymbol{a})^{\mathrm{T}}$ and $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\boldsymbol{a}')^{\mathrm{T}}$ are represented by rows [indicated by $(\ldots)^{\mathrm{T}}$, which means 'transposed']. The quantities with unprimed symbols are referred to the coordinate system of $\mathcal{G}$, those with primes are referred to the coordinate system of $\mathcal{H}$.

The following columns will be used ($\boldsymbol{w}'$ is analogous to $\boldsymbol{w}$):

$$\boldsymbol{w}=\begin{pmatrix}w_1\\w_2\\w_3\end{pmatrix};\ \boldsymbol{x}=\begin{pmatrix}x\\y\\z\end{pmatrix};\ \boldsymbol{x}'=\begin{pmatrix}x'\\y'\\z'\end{pmatrix};\ \boldsymbol{p}=\begin{pmatrix}p_1\\p_2\\p_3\end{pmatrix};\ \boldsymbol{q}=\begin{pmatrix}q_1\\q_2\\q_3\end{pmatrix}.$$

The (3×3) matrices $\boldsymbol{W}$ and $\boldsymbol{W}'$ of the symmetry operations, as well as the matrix $\boldsymbol{P}$ for a change of basis and its inverse $\boldsymbol{Q}=\boldsymbol{P}^{-1}$, are designated by boldface italic upper-case letters ($\boldsymbol{W}'$ is analogous to $\boldsymbol{W}$):

$$\boldsymbol{W}=\begin{pmatrix}W_{11}\,W_{12}\,W_{13}\\W_{21}\,W_{22}\,W_{23}\\W_{31}\,W_{32}\,W_{33}\end{pmatrix};\ \boldsymbol{P}=\begin{pmatrix}P_{11}\,P_{12}\,P_{13}\\P_{21}\,P_{22}\,P_{23}\\P_{31}\,P_{32}\,P_{33}\end{pmatrix};\ \boldsymbol{Q}=\begin{pmatrix}Q_{11}\,Q_{12}\,Q_{13}\\Q_{21}\,Q_{22}\,Q_{23}\\Q_{31}\,Q_{32}\,Q_{33}\end{pmatrix}.$$

Let $\mathbf{a},\mathbf{b},\mathbf{c}=(\boldsymbol{a})^{\mathrm{T}}$ be the row of basis vectors of $\mathcal{G}$ and $\mathbf{a}',\mathbf{b}',\mathbf{c}'=(\boldsymbol{a}')^{\mathrm{T}}$ the basis of $\mathcal{H}$, then the basis $(\boldsymbol{a}')^{\mathrm{T}}$ is expressed in the basis $(\boldsymbol{a})^{\mathrm{T}}$ by the system of equations[2]

$$\begin{aligned}\mathbf{a}'&=P_{11}\,\mathbf{a}+P_{21}\,\mathbf{b}+P_{31}\,\mathbf{c}\\\mathbf{b}'&=P_{12}\,\mathbf{a}+P_{22}\,\mathbf{b}+P_{32}\,\mathbf{c}\\\mathbf{c}'&=P_{13}\,\mathbf{a}+P_{23}\,\mathbf{b}+P_{33}\,\mathbf{c}\end{aligned}\qquad(2.1.3.1)$$

or

$$(\mathbf{a}',\mathbf{b}',\mathbf{c}')^{\mathrm{T}}=(\mathbf{a},\mathbf{b},\mathbf{c})^{\mathrm{T}}\begin{pmatrix}P_{11}\,P_{12}\,P_{13}\\P_{21}\,P_{22}\,P_{23}\\P_{31}\,P_{32}\,P_{33}\end{pmatrix}.\qquad(2.1.3.2)$$

In matrix notation, this is

$$(\boldsymbol{a}')^{\mathrm{T}}=(\boldsymbol{a})^{\mathrm{T}}\boldsymbol{P}.\qquad(2.1.3.3)$$

The column $\boldsymbol{p}$ of coordinates of the origin O' of $\mathcal{H}$ is referred to the coordinate system of $\mathcal{G}$ and is called the *origin shift*. The matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$ describes the transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$, for details, *cf.* *IT* A, Part 5. Therefore, $\boldsymbol{P}$ and $\boldsymbol{p}$ are chosen in the subgroup tables in the columns 'matrix' and 'shift', *cf.* Section 2.1.3.2. The column 'matrix' is empty if there is no change of basis, *i.e.* if $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$. The column 'shift' is empty if there is no origin shift, *i.e.* if $\boldsymbol{p}$ is the column $\boldsymbol{o}$ consisting of zeroes only.

A change of the coordinate system, described by the matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$, changes the point coordinates from the column $\boldsymbol{x}$ to the column $\boldsymbol{x}'$. The formulae for this change do not contain the pair $(\boldsymbol{P},\boldsymbol{p})$ itself, but the related pair $(\boldsymbol{Q},\ \boldsymbol{q})=(\boldsymbol{P}^{-1},\ -\boldsymbol{P}^{-1}\boldsymbol{p})$:

$$\boldsymbol{x}'=\boldsymbol{Q}\boldsymbol{x}+\boldsymbol{q}=\boldsymbol{P}^{-1}\boldsymbol{x}-\boldsymbol{P}^{-1}\boldsymbol{p}=\boldsymbol{P}^{-1}(\boldsymbol{x}-\boldsymbol{p}).\qquad(2.1.3.4)$$

Not only the point coordinates but also the matrix–column pairs for the symmetry operations are changed by a change of the coordinate system. A symmetry operation W is described in the coordinate system of $\mathcal{G}$ by the system of equations

$$\begin{aligned}\tilde{x}&=W_{11}\,x+W_{12}\,y+W_{13}\,z+w_1\\\tilde{y}&=W_{21}\,x+W_{22}\,y+W_{23}\,z+w_2\\\tilde{z}&=W_{31}\,x+W_{32}\,y+W_{33}\,z+w_3,\end{aligned}\qquad(2.1.3.5)$$

$$\tilde{\boldsymbol{x}}=\boldsymbol{W}\boldsymbol{x}+\boldsymbol{w}=(\boldsymbol{W},\boldsymbol{w})\,\boldsymbol{x},\qquad(2.1.3.6)$$

i.e. by the matrix–column pair $(\boldsymbol{W},\boldsymbol{w})$. The symmetry operation W will be described in the coordinate system of the subgroup $\mathcal{H}$ by the equation

$$\tilde{\boldsymbol{x}}'=\boldsymbol{W}'\boldsymbol{x}'+\boldsymbol{w}'=(\boldsymbol{W}',\ \boldsymbol{w}')\,\boldsymbol{x}',\qquad(2.1.3.7)$$

and thus by the pair $(\boldsymbol{W}',\ \boldsymbol{w}')$. This pair can be calculated from the pair $(\boldsymbol{W},\ \boldsymbol{w})$ by solving the equations

$$\boldsymbol{W}'=\boldsymbol{Q}\,\boldsymbol{W}\boldsymbol{P}=\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\qquad(2.1.3.8)$$

and

$$\boldsymbol{w}'=\boldsymbol{q}+\boldsymbol{Q}\boldsymbol{w}+\boldsymbol{Q}\boldsymbol{W}\boldsymbol{p}=\boldsymbol{P}^{-1}(\boldsymbol{w}+\boldsymbol{W}\boldsymbol{p}-\boldsymbol{p})=\boldsymbol{P}^{-1}(\boldsymbol{w}+(\boldsymbol{W}-\boldsymbol{I})\boldsymbol{p}).\qquad(2.1.3.9)$$

Example 2.1.3.3.1.

Consider the data listed for the *t*-subgroups of $Pmn2_1$, No. 31:

Index	HM & No.	sequence	matrix	shift
[2]	$P1n1$ (7, $P1c1$)	1; 3	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2]	$Pm11$ (6, $P1m1$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2]	$P112_1$ (4)	1; 2		$1/4, 0, 0$

This means that the matrices and origin shifts are

(1) $$\boldsymbol{P}_1=\begin{pmatrix}0&0&\bar{1}\\0&1&0\\1&0&\bar{1}\end{pmatrix};\boldsymbol{P}_2=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix};\boldsymbol{P}_3=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$$

(2) $$\boldsymbol{p}_1=\begin{pmatrix}0\\0\\0\end{pmatrix},\ \boldsymbol{p}_2=\begin{pmatrix}0\\0\\0\end{pmatrix},\ \boldsymbol{p}_3=\begin{pmatrix}\frac{1}{4}\\0\\0\end{pmatrix}.$$

(3) The first subgroup is monoclinic, the symmetry direction is the *b* axis, which is standard. However, the glide direction $\frac{1}{2}(\mathbf{a}+\mathbf{c})$ is nonconventional. Therefore, the basis of $\mathcal{G}$ is transformed to a basis of the subgroup $\mathcal{H}$ such that the *b* axis is retained, the glide direction becomes the c' axis and the a' axis is chosen such that the basis is a right-handed one, the angle $\beta'\geq 90°$ and the transformation matrix $\boldsymbol{P}$ is simple. This is done by the chosen matrix $\boldsymbol{P}_1$. The origin shift is the $\boldsymbol{o}$ column.
With equations (2.1.3.8) and (2.1.3.9), one obtains for the glide reflection $x,\bar{y},z-\frac{1}{2}$, which is $x,\bar{y},z+\frac{1}{2}$ after standardization by $0\leq w_j<1$.

(4) For the second monoclinic subgroup, the symmetry direction is the (nonconventional) *a* axis. The rules of Section 2.1.2.5 require a change to the setting 'unique axis *b*'. A cyclic permutation of the basis vectors is the simplest way to achieve this. The reflection $\bar{x},y,z$ is now described by $x,\bar{y},z$. Again there is no origin shift.

(5) The third monoclinic subgroup is in the conventional setting 'unique axis *c*', but the origin must be shifted onto the 2_1 screw axis. This is achieved by applying equation (2.1.3.9) with $\boldsymbol{p}_3$, which changes $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ of $Pmn2_1$ to $\bar{x},\bar{y},z+\frac{1}{2}$ of $P112_1$.

Example 2.1.3.3.2.

Evaluation of the *t*-subgroup data of the space group $P3_112$, No. 151, started in Example 2.1.3.2.4. The evaluation is now continued with the columns 'sequence', 'matrix' and 'shift'. They are used for the transformation of the elements of $\mathcal{H}$ to their conventional form. Only the monoclinic *t*-subgroups are of interest here because the trigonal subgroup is already in the standard setting.

[2] The system of equations (2.1.3.1) is similar but not identical to the system of equations (2.1.3.5), which describes a symmetry operation W by the matrix $\boldsymbol{W}$ and the column $\boldsymbol{w}$. Both $\boldsymbol{W}$ and $\boldsymbol{w}$ are listed as the general position in the space-group tables of *IT* A, *cf.* Part 5 and Chapter 11.2 of *IT* A. The essential difference is that in equation (2.1.3.6) the matrix $\boldsymbol{W}$ is multiplied by the column $\boldsymbol{x}$ from the *right-hand* side whereas in equation (2.1.3.3) the matrix $\boldsymbol{P}$ is multiplied by the row $(\boldsymbol{a})^{\mathrm{T}}$ from the *left-hand* side. Therefore, the running index in $\boldsymbol{W}$ is the second one, whereas in $\boldsymbol{P}$ it is the first one.

One takes from the tables of subgroups in Chapter 2.3

Index	HM & No.	sequence	matrix	shift
[3]	$P112$ (5, $C121$)	1; 6	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	
[3]	$P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	0, 0, 1/3
[3]	$P112$ (5, $C121$)	1; 5	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	0, 0, 2/3

Designating the three matrices by $\boldsymbol{P}_6, \boldsymbol{P}_4, \boldsymbol{P}_5$, one obtains

$$\boldsymbol{P}_6 = \begin{pmatrix} 0 & -2 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{P}_4 = \begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{P}_5 = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with the corresponding inverse matrices

$$\boldsymbol{Q}_6 = \begin{pmatrix} -\frac{1}{2} & 1 & 0 \\ -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{Q}_4 = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{Q}_5 = \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the origin shifts

$$\boldsymbol{p}_6 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{p}_4 = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}, \ \boldsymbol{p}_5 = \begin{pmatrix} 0 \\ 0 \\ \frac{2}{3} \end{pmatrix}.$$

For the three new bases this means

$$\begin{aligned} &\mathbf{a}'_6 = \mathbf{b}, \ \mathbf{b}'_6 = -2\mathbf{a} - \mathbf{b}, \ \mathbf{c}'_6 = \mathbf{c} \\ &\mathbf{a}'_4 = -\mathbf{a} - \mathbf{b}, \ \mathbf{b}'_4 = \mathbf{a} - \mathbf{b}, \ \mathbf{c}'_4 = \mathbf{c} \text{ and} \\ &\mathbf{a}'_5 = \mathbf{a}, \ \mathbf{b}'_5 = \mathbf{a} + 2\mathbf{b}, \ \mathbf{c}'_5 = \mathbf{c}. \end{aligned}$$

All these bases span ortho-hexagonal cells with twice the volume of the original hexagonal cell because for the matrices $\det(\boldsymbol{P}_i) = 2$ holds.
In the general position of $\mathcal{G} = P3_112$, No.151, one finds

(1) x, y, z; (4) $\bar{y}, \bar{x}, \bar{z} + \frac{2}{3}$; (5) $\bar{x} + y, y, \bar{z} + \frac{1}{3}$; (6) $x, x - y, \bar{z}$.

These entries represent the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$:

$$(1) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4) \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{2}{3} \end{pmatrix};$$

$$(5) \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}; \quad (6) \begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Application of equations (2.1.3.8) on the matrices $\boldsymbol{W}_k$ and (2.1.3.9) on the columns $\boldsymbol{w}_k$ of the matrix–column pairs results in

$$\boldsymbol{W}'_4 = \boldsymbol{W}'_5 = \boldsymbol{W}'_6 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}; \ \boldsymbol{w}'_4 = \boldsymbol{w}'_6 = \boldsymbol{o}; \ \boldsymbol{w}'_5 = \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix}.$$

All translation vectors of $\mathcal{G}$ are retained in the subgroups but the volume of the cells is doubled. Therefore, there must be centring-translation vectors in the new cells. For example, the application of equation (2.1.3.9) with $(\boldsymbol{P}_6, \boldsymbol{p}_6)$ to the translation of $\mathcal{G}$ with the vector $-\mathbf{a}$, *i.e.* $\boldsymbol{w} = -(1, 0, 0)$, results in the column $\boldsymbol{w}' = (\frac{1}{2}, \frac{1}{2}, 0)$, *i.e.* the centring translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}')$ of the subgroup. Either by calculation or, more easily, from a small sketch one sees that the vectors $-\mathbf{b}$ for $\boldsymbol{P}_4$, $\mathbf{a} + \mathbf{b}$ for $\boldsymbol{P}_5$ (and $-\mathbf{a}$ for $\boldsymbol{P}_6$) correspond to the cell-centring translation vectors of the subgroup cells.

Comments:

This example reveals that the conjugation of conjugate subgroups does not necessarily imply the conjugation of the representatives of these subgroups in the general positions of *IT* A. The three monoclinic subgroups $C121$ in this example are conjugate in the group $\mathcal{G}$ by the 3_1 screw rotation. Conjugation of the representative (4) by the 3_1 screw rotation of $\mathcal{G}$ results in the representative (5) with the column $\boldsymbol{w}_5 = 0, 0, \frac{4}{3}$, which is not exactly the representative (5) but one of its translationally equivalent elements of $\mathcal{G}$ retained in $\mathcal{H}$.

2.1.4. II Maximal *klassengleiche* subgroups (*k*-subgroups)

2.1.4.1. *General description*

The listing of the maximal *klassengleiche* subgroups (maximal *k*-subgroups) $\mathcal{H}_j$ of the space group $\mathcal{G}$ is divided into the following three blocks for practical reasons:

• **Loss of centring translations**. Maximal subgroups $\mathcal{H}$ of this block have the same conventional unit cell as the original space group $\mathcal{G}$. They are always non-isomorphic and have index 2 for plane groups and index 2, 3 or 4 for space groups.

• **Enlarged unit cell**. Under this heading, maximal subgroups of index 2, 3 and 4 are listed for which the *conventional* unit cell has been enlarged. The block contains isomorphic *and* non-isomorphic subgroups with this property.

• **Series of maximal isomorphic subgroups**. In this block *all* maximal isomorphic subgroups of a space group $\mathcal{G}$ are listed in a small number of infinite series of subgroups with no restriction on the index, *cf.* Sections 2.1.2.4 and 2.1.5.

The description of the subgroups is the same within the same block but differs between the blocks. The partition into these blocks differs from the partition in *IT* A, where the three blocks are called 'maximal non-isomorphic subgroups IIa', 'maximal non-isomorphic subgroups IIb' and 'maximal isomorphic subgroups of lowest index IIc'.

The kind of listing in the three blocks of this volume is discussed in Sections 2.1.4.2, 2.1.4.3 and 2.1.5 below.

2.1.4.2. *Loss of centring translations*

Consider a space group $\mathcal{G}$ with a centred lattice, *i.e.* a space group whose HM symbol does not start with the lattice letter P but with one of the letters A, B, C, F, I or R. The block contains those maximal subgroups of $\mathcal{G}$ which have fully or partly lost their centring translations and thus are not *t*-subgroups. The *conventional* unit cell is *not* changed.

Only in space groups with an F-centred lattice can the centring be partially lost, as is seen in the list of the space group $Fmmm$, No. 69. On the other hand, for $F23$, No. 196, the maximal subgroups $P23$, No. 195, or $P2_13$, No. 198, have lost all their centring translations.

For the block 'Loss of centring translations', the listing in this volume is the same as that for *t*-subgroups, *cf.* Section 2.1.3. The centring translations are listed explicitly where applicable, *e.g.* for space group $C2$, No. 5, unique axis b

[2] $P12_11$ (4) 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$ 1/4, 0, 0.

In this line, the representatives 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$ of the general position are x, y, z $\ \bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$.

references