International Tables for Crystallography (2011). Vol. A1, Section 2.1.3.3, pp. 77–79.

Comments:
HMS1: The sequence of the directions 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 2.1.3.2.5
$\mathcal{G} = P3_112$, No. 151
I Maximal *translationengleiche* subgroups

[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**a** − **b**, **a** − **b** and **a** + 2**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. The transformation described in this section is not restricted to *translationengleiche* subgroups but is applied to *klassengleiche* subgroups as well.

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

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

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 listed 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[2]

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

or

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

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

[2] Please note 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.

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

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

$$\boldsymbol{W}' = \boldsymbol{Q}\,\boldsymbol{W}\,\boldsymbol{P} = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \tag{2.1.3.8}$$

and

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

These equations are rather complicated and unpleasant. They become simple when using augmented matrices and columns. In this case the formulae are reduced formally to normal matrix multiplication [the formalism is simpler but the necessary calculations are not, because the inversion of a (4 × 4) matrix is tedious if done by hand].

The matrices $\boldsymbol{P}$, $\boldsymbol{Q}$, $\boldsymbol{W}$ and $\boldsymbol{W}'$ may be combined with the corresponding columns $\boldsymbol{p}$, $\boldsymbol{q}$, $\boldsymbol{w}$ and $\boldsymbol{w}'$ to form (4 × 4) matrices (callled *augmented matrices*):[3]

$$\mathbb{P} = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{Q} = \mathbb{P}^{-1} = \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W}' = \left(\begin{array}{ccc|c} W'_{11} & W'_{12} & W'_{13} & w'_1 \\ W'_{21} & W'_{22} & W'_{23} & w'_2 \\ W'_{31} & W'_{32} & W'_{33} & w'_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

The coefficients of these augmented matrices are integer, rational or real numbers.

The (3 × 1) rows $(\boldsymbol{a})^{\rm T}$ and $(\boldsymbol{a}')^{\rm T}$ must be augmented to (4 × 1) rows by appending some vectors $\mathbf{s}_{\mathcal{G}}$ and $\mathbf{s}'_{\mathcal{H}}$, respectively, as fourth entries in order to enable matrix multiplication with the augmented matrices:

$$(\mathbb{a})^{\rm T} = (\mathbf{a}, \mathbf{b}, \mathbf{c} \mid \mathbf{s}_{\mathcal{G}})^{\rm T} \quad \text{and} \quad (\mathbb{a}')^{\rm T} = (\mathbf{a}', \mathbf{b}', \mathbf{c}' \mid \mathbf{s}'_{\mathcal{H}})^{\rm T}$$

with $\mathbf{s}'_{\mathcal{H}} = \mathbf{p} + \mathbf{s}_{\mathcal{G}}$. As the vector $\mathbf{s}_{\mathcal{G}}$ one can take the zero vector $\mathbf{s}_{\mathcal{G}} = \mathbf{o}$, which results in $\mathbf{s}'_{\mathcal{H}} = \mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}$, *i.e.*

$$(\mathbb{a})^{\rm T} = (\mathbf{a}, \mathbf{b}, \mathbf{c} \mid \mathbf{o})^{\rm T} \quad \text{and} \quad (\mathbb{a}')^{\rm T} = (\mathbf{a}', \mathbf{b}', \mathbf{c}' \mid \mathbf{p})^{\rm T}.$$

The relation between $(\mathbb{a}')^{\rm T}$ and $(\mathbb{a})^{\rm T}$ is given by equation (2.1.3.10), which replaces equation (2.1.3.3),

$$(\mathbb{a}')^{\rm T} = (\mathbb{a})^{\rm T}\mathbb{P}. \tag{2.1.3.10}$$

Analogously, the (3 × 1) columns $\boldsymbol{x}$ and $\boldsymbol{x}'$ must be augmented to (4 × 1) columns by a '1' in the fourth row in order to enable matrix multiplication with the augmented matrices:

$$\mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right); \quad \mathbb{x}' = \left(\begin{array}{c} x' \\ y' \\ z' \\ \hline 1 \end{array}\right).$$

The three equations (2.1.3.4), (2.1.3.8) and (2.1.3.9) are replaced by the two equations

$$\mathbb{x}' = \mathbb{Q}\mathbb{x} = \mathbb{P}^{-1}\mathbb{x} \tag{2.1.3.11}$$

and

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P} = \mathbb{P}^{-1}\mathbb{W}\mathbb{P}. \tag{2.1.3.12}$$

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	**c**, **b**, −**a** − **c**	
[2]	$Pm11$ (6, $P1m1$)	1; 4	**c**, **a**, **b**	
[2]	$P112_1$ (4)	1; 2		1/4, 0, 0

This means that the transformation matrices and origin shifts are

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

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

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 $0 \leq w_j < 1$.

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.

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 2.1.3.2.5. 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

[3] The horizontal and vertical lines in the augmented matrices are useful to facilitate recognition of their coefficients; they have no mathematical meaning.

of interest here because the trigonal subgroup is already in the standard setting.

One takes from the tables of subgroups in Chapter 2.3

Index	HM & No.	sequence	matrix	shift
[3]	*P*112 (5, *C*121)	1; 6	**b**, −2**a** − **b**, **c**	
[3]	*P*112 (5, *C*121)	1; 4	−**a** − **b**, **a** − **b**, **c**	0, 0, 1/3
[3]	*P*112 (5, *C*121)	1; 5	**a**, **a** + 2**b**, **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

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

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

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

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 *C*121 in this example are conjugate in the group $\mathcal{G}$ by the 3_1 screw rotation. Conjugation of the representatives (4) and (6) by the 3_1 screw rotation of $\mathcal{G}$ results in the column $\boldsymbol{w}_5 = 0, 0, \frac{4}{3}$, which is standardized according to the rules of *IT* A to $\boldsymbol{w}_5 = 0, 0, \frac{1}{3}$. Thus, the conjugacy relation is disturbed by the standardization of the representative (5).

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) $\mathcal{H}$ 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 *F*23, No. 196, the maximal subgroups *P*23, 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 *C*2, 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 $x, y, z \quad \bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$.