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

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

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) $\bar{y}, \bar{x}, \bar{z} + \frac{2}{3}$; (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