International Tables for Crystallography (2006). Vol. A1, Section 2.1.4, pp. 48–51.

One takes from the tables of subgroups in Chapter 2.3

Index	HM & No.	sequence	matrix	shift
[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

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 $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$.

The listing differs from that in *IT* A in only two points:

(1) the full HM symbol is taken as the conventional symbol for monoclinic space groups, whereas in *IT* A the short HM symbol is the conventional one;

(2) the information needed for the transformation of the data from the setting of the space group $\mathcal{G}$ to that of $\mathcal{H}$ is added. In this example, the matrix is the unit matrix and is not listed; the column of origin shift is $\frac{1}{4}, 0, 0$. This transformation is analogous to that of *t*-subgroups and is described in detail in Section 2.1.3.3.

The sequence of the subgroups in this block is one of decreasing space-group number of the subgroups.

2.1.4.3. *Enlarged unit cell*

Under the heading 'Enlarged unit cell', those maximal *k*-subgroups $\mathcal{H}$ are listed for which the conventional unit cell is enlarged relative to the unit cell of the original space group $\mathcal{G}$. *All* maximal *k*-subgroups with enlarged unit cell of index 2, 3 or 4 of the plane groups and of the space groups are listed *individually*. The listing is restricted to these indices because 4 is the highest index of a maximal *non-isomorphic* subgroup, and the number of these subgroups is finite. Maximal subgroups of higher indices are always isomorphic to $\mathcal{G}$ and their number is infinite.

The description of the subgroups with enlarged unit cell is more detailed than in *IT* A. In the block IIb of *IT* A, different maximal subgroups of the same space-group type with the same lattice relations are represented by the same entry. For example, the eight maximal subgroups of the type *Fmmm*, No. 69, of space group *Pmmm*, No. 47, are represented by one entry in *IT* A.

In the present volume, the description of the maximal subgroups in the block 'Enlarged unit cell' refers to each subgroup individually and contains for each of them a set of space-group generators and the transformation from the setting of the space group $\mathcal{G}$ to the conventional setting of the subgroup $\mathcal{H}$.

Some of the isomorphic subgroups listed in this block may also be found in *IT* A in the block 'Maximal isomorphic subgroups of lowest index IIc'.

Subgroups with the same lattice are collected in small blocks. The heading of each such block consists of the index of the subgroup and the lattice relations of the sublattice relative to the original lattice. Basis vectors that are not mentioned are not changed.

Example 2.1.4.3.1.

This example is taken from the table of space group $C222_1$, No. 20.

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$

$$\left\{\begin{array}{llll} C222_1 & (20) & \langle 2;3\rangle & 3\mathbf{a},\mathbf{b},\mathbf{c} & \\ C222_1 & (20) & \langle (2;3)+(2,0,0)\rangle & 3\mathbf{a},\mathbf{b},\mathbf{c} & 1,0,0 \\ C222_1 & (20) & \langle (2;3)+(4,0,0)\rangle & 3\mathbf{a},\mathbf{b},\mathbf{c} & 2,0,0 \end{array}\right.$$

[3] $\mathbf{b}' = 3\mathbf{b}$

$$\left\{\begin{array}{llll} C222_1 & (20) & \langle 2;3\rangle & \mathbf{a},3\mathbf{b},\mathbf{c} & \\ C222_1 & (20) & \langle 3;2+(0,2,0)\rangle & \mathbf{a},3\mathbf{b},\mathbf{c} & 0,1,0 \\ C222_1 & (20) & \langle 3;2+(0,4,0)\rangle & \mathbf{a},3\mathbf{b},\mathbf{c} & 0,2,0 \end{array}\right.$$

The entries mean:

Columns 1 and 2: HM symbol and space-group number of the subgroup; *cf.* Section 2.1.3.2.

Column 3: generators, here the pairs

$$\begin{array}{ll} \bar{x},\bar{y},z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \\ \bar{x}+2,\bar{y},z+\frac{1}{2}; & \bar{x}+2,y,\bar{z}+\frac{1}{2}; \\ \bar{x}+4,\bar{y},z+\frac{1}{2}; & \bar{x}+4,y,\bar{z}+\frac{1}{2}; \end{array}$$

$$\begin{array}{ll} \bar{x},\bar{y},z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \\ \bar{x},\bar{y}+2,z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \\ \bar{x},\bar{y}+4,z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \end{array}$$

for the six lines listed in the same order.

Column 4: basis vectors of $\mathcal{H}$ referred the basis vectors of $\mathcal{G}$. $3\mathbf{a},\mathbf{b},\mathbf{c}$ means $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$; $\mathbf{a},3\mathbf{b},\mathbf{c}$ means $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

Column 5: origin shifts, referred to the coordinate system of $\mathcal{G}$. These origin shifts by $\mathbf{o}$, $\mathbf{a}$ and $2\mathbf{a}$ for the first triplet of subgroups and $\mathbf{o}$, $\mathbf{b}$ and $2\mathbf{b}$ for the second triplet of subgroups are translations of $\mathcal{G}$. The subgroups of each triplet are conjugate, indicated by the left braces.

Often the lattice relations above the data describing the subgroups are the same as the basis vectors in column 4, as in this example. They differ in particular if the sublattice of $\mathcal{H}$ is non-conventionally centred. Examples are the *H*-centred subgroups of trigonal and hexagonal space groups.

The sequence of the subgroups is determined

(1) by the index of the subgroup such that the subgroups of lowest index are given first;
(2) within the same index by the kind of cell enlargement;
(3) within the same cell enlargement by the No. of the subgroup, such that the subgroup of highest space-group number is given first.

2.1.4.3.1. *Enlarged unit cell, index 2*

For sublattices with twice the volume of the unit cell, the sequence of the different cell enlargements is as follows:

(1) Triclinic space groups:

(i) $\mathbf{a}' = 2\mathbf{a}$,
(ii) $\mathbf{b}' = 2\mathbf{b}$,
(iii) $\mathbf{c}' = 2\mathbf{c}$,
(iv) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
(v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
(vi) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
(vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.

(2) Monoclinic space groups:

(*a*) with *P* lattice, unique axis *b*:

(i) $\mathbf{b}' = 2\mathbf{b}$,
(ii) $\mathbf{c}' = 2\mathbf{c}$,
(iii) $\mathbf{a}' = 2\mathbf{a}$,
(iv) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
(v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
(vi) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
(vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.

(*b*) with *P* lattice, unique axis *c*:

(i) $\mathbf{c}' = 2\mathbf{c}$,
(ii) $\mathbf{a}' = 2\mathbf{a}$,
(iii) $\mathbf{b}' = 2\mathbf{b}$,
(iv) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
(v) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
(vi) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
(vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.

(*c*) with C lattice, unique axis b: There are three sublattices of index 2 of a monoclinic C lattice. One has lost its centrings such that a P lattice with the same unit cell remains. The subgroups with this sublattice are listed under 'Loss of centring translations'. The block with the other two sublattices consists of $\mathbf{c}' = 2\mathbf{c}$, C-centring and I-centring. The sequence of the subgroups in this block is determined by the space-group number of the subgroup.

(*d*) with A lattice, unique axis c: There are three sublattices of index 2 of a monoclinic A lattice. One has lost its centrings such that a P lattice with the same unit cell remains. The subgroups with this sublattice are listed under 'Loss of centring translations'. The block with the other two sublattices consists of $\mathbf{a}' = 2\mathbf{a}$, A-centring and I-centring. The sequence of the subgroups in this block is determined by the No. of the subgroup.

(3) Orthorhombic space groups:

(*a*) Orthorhombic space groups with P lattice: Same sequence as for triclinic space groups.

(*b*) Orthorhombic space groups with C (or A) lattice: Same sequence as for monoclinic space groups with C (or A) lattice.

(*c*) Orthorhombic space groups with I and F lattice: There are no subgroups of index 2 with enlarged unit cell.

(4) Tetragonal space groups:

(*a*) Tetragonal space groups with P lattice:

(i) $\mathbf{c}' = 2\mathbf{c}$.

(ii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$, C-centring. The conventional setting results in a P lattice.

(iii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, F-centring. The conventional setting results in an I lattice.

(*b*) Tetragonal space groups with I lattice: There are no subgroups of index 2 with enlarged unit cell.

(5) For trigonal and hexagonal space groups, $\mathbf{c}' = 2\mathbf{c}$ holds.
For rhombohedral space groups referred to hexagonal axes, $\mathbf{a}' = -\mathbf{b},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b},\ \mathbf{b}' = -\mathbf{a},\ \mathbf{c}' = 2\mathbf{c}$ holds.
For rhombohedral space groups referred to rhombohedral axes, $\mathbf{a}' = \mathbf{a}+\mathbf{c},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = \mathbf{b}+\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, F-centring holds.

(6) Only cubic space groups with a P lattice have subgroups of index 2 with enlarged unit cell. For their lattices the following always holds: $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, F-centring.

2.1.4.3.2. *Enlarged unit cell, index 3 or 4*

With a few exceptions for trigonal, hexagonal and cubic space groups, k-subgroups with enlarged unit cells and index 3 or 4 are isomorphic. To each of the listed sublattices belong either one or several conjugacy classes with three or four conjugate subgroups or one or several normal subgroups. Only the sublattices with the numbers (5)(*a*)(v), (5)(*b*)(i), (5)(*c*)(ii), (6)(iii) and (7)(i) have index 4, all others have index 3. The different cell enlargements are listed in the following sequence:

(1) Triclinic space groups:

(i) $\mathbf{a}' = 3\mathbf{a}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = \mathbf{a}+\mathbf{b}$,

(iii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 2\mathbf{a}+\mathbf{b}$,

(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{c}' = \mathbf{a}+\mathbf{c}$,

(v) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$,

(vi) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = \mathbf{a}+\mathbf{c}$,

(vii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 2\mathbf{a}+\mathbf{b},\ \mathbf{c}' = \mathbf{a}+\mathbf{c}$,

(viii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$,

(ix) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 2\mathbf{a}+\mathbf{b},\ \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$,

(x) $\mathbf{b}' = 3\mathbf{b}$,

(xi) $\mathbf{b}' = 3\mathbf{b},\ \mathbf{c}' = \mathbf{b}+\mathbf{c}$,

(xii) $\mathbf{b}' = 3\mathbf{b},\ \mathbf{c}' = 2\mathbf{b}+\mathbf{c}$,

(xiii) $\mathbf{c}' = 3\mathbf{c}$.

(2) Monoclinic space groups:

(*a*) Space groups $P121$, $P12_11$, $P1m1$, $P12/m1$, $P12_1/m1$ (unique axis b):

(i) $\mathbf{b}' = 3\mathbf{b}$,

(ii) $\mathbf{c}' = 3\mathbf{c}$,

(iii) $\mathbf{a}' = \mathbf{a}-\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$,

(iv) $\mathbf{a}' = \mathbf{a}-2\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$,

(v) $\mathbf{a}' = 3\mathbf{a}$.

(*b*) Space groups $P112$, $P112_1$, $P11m$, $P112/m$, $P112_1/m$ (unique axis c):

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a}$,

(iii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -\mathbf{a}+\mathbf{b}$,

(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$,

(v) $\mathbf{b}' = 3\mathbf{b}$.

(*c*) Space groups $P1c1$, $P12/c1$, $P12_1/c1$ (unique axis b):

(i) $\mathbf{b}' = 3\mathbf{b}$,

(ii) $\mathbf{c}' = 3\mathbf{c}$,

(iii) $\mathbf{a}' = 3\mathbf{a}$,

(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{c}' = -2\mathbf{a}+\mathbf{c}$,

(v) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{c}' = -4\mathbf{a}+\mathbf{c}$.

(*d*) Space groups $P11a$, $P112/a$, $P112_1/a$ (unique axis c):

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a}$,

(iii) $\mathbf{b}' = 3\mathbf{b}$,

(iv) $\mathbf{a}' = \mathbf{a}-2\mathbf{b},\ \mathbf{b}' = 3\mathbf{b}$,

(v) $\mathbf{a}' = \mathbf{a}-4\mathbf{b},\ \mathbf{b}' = 3\mathbf{b}$.

(*e*) All space groups with C lattice (unique axis b):

(i) $\mathbf{b}' = 3\mathbf{b}$,

(ii) $\mathbf{c}' = 3\mathbf{c}$,

(iii) $\mathbf{a}' = \mathbf{a}-2\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$,

(iv) $\mathbf{a}' = \mathbf{a}-4\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$,

(v) $\mathbf{a}' = 3\mathbf{a}$.

(*f*) All space groups with A lattice (unique axis c):

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a}$,

(iii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$,

(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -4\mathbf{a}+\mathbf{b}$,

(v) $\mathbf{b}' = 3\mathbf{b}$.

(3) Orthorhombic space groups:

(i) $\mathbf{a}' = 3\mathbf{a}$,

(ii) $\mathbf{b}' = 3\mathbf{b}$,

(iii) $\mathbf{c}' = 3\mathbf{c}$.

(4) Tetragonal space groups:

(i) $\mathbf{c}' = 3\mathbf{c}$.

(5) Trigonal space groups:

(*a*) Trigonal space groups with hexagonal *P* lattice:

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$, *H*-centring,

(iii) $\mathbf{a}' = \mathbf{a} - \mathbf{b},\ \mathbf{b}' = \mathbf{a} + 2\mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$, *R* lattice,

(iv) $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$, *R* lattice,

(v) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$.

(*b*) Trigonal space groups with rhombohedral *R* lattice and hexagonal axes:

(i) $\mathbf{a}' = -2\mathbf{b},\ \mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$.

(*c*) Trigonal space groups with rhombohedral *R* lattice and rhombohedral axes:

(i) $\mathbf{a}' = \mathbf{a} - \mathbf{b},\ \mathbf{b}' = \mathbf{b} - \mathbf{c},\ \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$,

(ii) $\mathbf{a}' = \mathbf{a} - \mathbf{b} + \mathbf{c},\ \mathbf{b}' = \mathbf{a} + \mathbf{b} - \mathbf{c},\ \mathbf{c}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}$.

(6) Hexagonal space groups:

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$, *H*-centring,

(iii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$.

(7) Cubic space groups with *P* lattice:

(i) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, *I* lattice.

2.1.5. Series of maximal isomorphic subgroups

By Y. Billiet

2.1.5.1. *General description*

Maximal subgroups of index higher than 4 have index p, p^2 or p^3, where p is prime, are necessarily isomorphic subgroups and are infinite in number. Only a few of them are listed in *IT* A in the block 'Maximal isomorphic subgroups of lowest index IIc'. Because of their infinite number, they cannot be listed individually, but are listed in this volume as members of series under the heading 'Series of maximal isomorphic subgroups'. In most of the series, the HM symbol for each isomorphic subgroup $\mathcal{H} < \mathcal{G}$ will be the same as that of $\mathcal{G}$. However, if $\mathcal{G}$ is an enantiomorphic space group, the HM symbol of $\mathcal{H}$ will be either that of $\mathcal{G}$ or that of its enantiomorphic partner.

Example 2.1.5.1.1.

Two of the four series of isomorphic subgroups of the space group $P4_1$, No. 76, are (the data on the generators are omitted):

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 2$; $p \equiv 3 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	$p > 4$; $p \equiv 1 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

On the other hand, the corresponding data for $P4_3$, No. 78, are

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 4$; $p \equiv 1 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	$p > 2$; $p \equiv 3 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

Note that in both tables the subgroups of the type $P4_3$, No. 78, are listed first because of the rules on the sequence of the subgroups.

If an isomorphic maximal subgroup of index $i \leq 4$ is a member of a series, then it is listed twice: as a member of its series *and* individually under the heading 'Enlarged unit cell'.

Most isomorphic subgroups of index 3 are the first members of series but those of index 2 or 4 are rarely so. An example is the space group $P4_2$, No. 77, with isomorphic subgroups of index 2 (not in any series) and 3 (in a series); an exception is found in space group $P4$, No. 75, where the isomorphic subgroup for $\mathbf{c}' = 2\mathbf{c}$ is the first member of the series $[p]\ \mathbf{c}' = p\mathbf{c}$.

2.1.5.2. *Basis transformation*

The conventional basis of the unit cell of each isomorphic subgroup in the series has to be defined relative to the basis of the original space group. For this definition the prime p is frequently sufficient as a parameter.

Example 2.1.5.2.1.

The isomorphic subgroups of the space group $P4_222$, No. 93, can be described by two series with the bases of their members:

$[p]$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
$[p^2]$	$p\mathbf{a},\ p\mathbf{b},\ \mathbf{c}$.

In other cases, one or two positive integers, here called q and r, define the series and often the value of the prime p.

Example 2.1.5.2.2.

In space group $P\overline{6}$, No. 174, the series $q\mathbf{a} - r\mathbf{b},\ r\mathbf{a} + (q + r)\mathbf{b},\ \mathbf{c}$ is listed. The values of q and r have to be chosen such that while $q > 0,\ r > 0,\ p = q^2 + r^2 + qr$ and p is prime.

Example 2.1.5.2.3.

In the space group $P112_1/m$, No. 11, unique axis c, the series $p\mathbf{a},\ -q\mathbf{a} + \mathbf{b},\ \mathbf{c}$ is listed. Here p and q are independent and q may take the p values $0 \leq q < p$ for each value of p.

2.1.5.3. *Origin shift*

Each of the sublattices discussed in Section 2.1.4.3.2 is common to a conjugacy class or belongs to a normal subgroup of a given series. The subgroups in a conjugacy class differ by the positions of their conventional origins relative to the origin of the space group $\mathcal{G}$. To define the origin of the conventional unit cell of each subgroup in a conjugacy class, one, two or three integers, called u, v or w in these tables, are necessary. For a series of subgroups of index p, p^2 or p^3 there are p, p^2 or p^3 conjugate subgroups, respectively. The positions of their origins are defined by the p or p^2 or p^3 permitted values of u or u, v or u, v, w, respectively.

Example 2.1.5.3.1.

The space group $\mathcal{G}$, $P\overline{4}2c$, No. 112, has two series of maximal isomorphic subgroups $\mathcal{H}$. For one of them the lattice relations are $[p^2]\ \mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$, listed as $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ for the transformation matrix. The index is p^2. For each value of p there exist exactly p^2 conjugate subgroups with origins in the points $u,\ v,\ 0$, where the parameters u and v run independently: $0 \leq u < p$ and $0 \leq v < p$.

In another type of series there is exactly one (normal) subgroup $\mathcal{H}$ for each index p; the location of its origin is always chosen at the origin $0, 0, 0$ of $\mathcal{G}$ and is thus not indicated as an origin shift.

Example 2.1.5.3.2.

Consider the space group $Pca2_1$, No. 29. Only one subgroup exists for each value of p in the series $\mathbf{a}, \mathbf{b}, p\mathbf{c}$. This is indicated in the tables by the statement 'no conjugate subgroups'.