International Tables for Crystallography (2006). Vol. A1, Section 2.1.4.3.1, pp. 49–50.

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

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

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

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

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