same or of the enantiomorphic space-group type as $\mathcal{G}$. The kind of listing is the same as for block **IIb**. Again, one entry may correspond to more than one isomorphic subgroup.

As the number of maximal isomorphic subgroups of a space group is always infinite, the data in block **IIc** are restricted to the subgroups of lowest index. Different kinds of cell enlargements are presented. For monoclinic, tetragonal, trigonal and hexagonal space groups, cell enlargements both parallel and perpendicular to the main rotation axis are listed; for orthorhombic space groups, this is the case for all three directions, *a*, *b* and *c*. Two isomorphic subgroups $\mathcal{H}_1$ and $\mathcal{H}_2$ of equal index but with cell enlargements in different directions may, nevertheless, play an analogous role with respect to $\mathcal{G}$. In terms of group theory, $\mathcal{H}_1$ and $\mathcal{H}_2$ then are conjugate subgroups in the affine normalizer of $\mathcal{G}$, *i.e.* they are mapped onto each other by automorphisms of $\mathcal{G}$.* Such subgroups are collected into one entry, with the different vector relationships separated by 'or' and placed within one pair of parentheses; *cf.* example (4).

*Examples*

(1) $\mathcal{G}$: $P\bar{3}1c$ (163)

**IIc** [3] $P\bar{3}1c$ ($\mathbf{c}' = 3\mathbf{c}$) (163); [4] $P\bar{3}1c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (163).

The first subgroup of index [3] entails an enlargement of the *c* axis, the second one of index [4] an enlargement of the mesh size in the *a*,*b* plane.

(2) $\mathcal{G}$: $P23$ (195)

**IIc** [27] $P23$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (195).

It seems surprising that [27] is the lowest index listed, even though another isomorphic subgroup of index [8] exists. The latter subgroup, however, is not maximal, as chains of maximal non-isomorphic subgroups can be constructed as follows:

$P23 \rightarrow [4]\ I23\ (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) \rightarrow [2]\ P23\ (\mathbf{a}', \mathbf{b}', \mathbf{c}')$

or

$P23 \rightarrow [2]\ F23\ (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) \rightarrow [4]\ P23\ (\mathbf{a}', \mathbf{b}', \mathbf{c}')$.

(3) $\mathcal{G}$: $P3_112$ (151)

**IIc** [2] $P3_212$ ($\mathbf{c}' = 2\mathbf{c}$) (153); [4] $P3_112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (151);
[7] $P3_112$ ($\mathbf{c}' = 7\mathbf{c}$) (151).

Note that the isomorphic subgroup of index [4] with $\mathbf{c}' = 4\mathbf{c}$ is not listed, because it is not maximal. This is apparent from the chain

$P3_112 \rightarrow [2]\ P3_212\ (\mathbf{c}' = 2\mathbf{c}) \rightarrow [2]\ P3_112\ (\mathbf{c}'' = 2\mathbf{c}' = 4\mathbf{c})$.

(4) $\mathcal{G}_1$: *Pnnm* (58)

**IIc** [3] *Pnnm* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (58); [3] *Pnnm* ($\mathbf{c}' = 3\mathbf{c}$) (58);

but $\mathcal{G}_2$: *Pnna* (52)

**IIc** [3] *Pnna* ($\mathbf{a}' = 3\mathbf{a}$) (52); [3] *Pnna* ($\mathbf{b}' = 3\mathbf{b}$) (52);
[3] *Pnna* ($\mathbf{c}' = 3\mathbf{c}$) (52).

For $\mathcal{G}_1 = Pnnm$, the *x* and *y* directions are analogous, *i.e.* they may be interchanged by automorphisms of $\mathcal{G}_1$. Such an automorphism does not exist for $\mathcal{G}_2 = Pnna$ because this space group contains glide reflections *a* but not *b*.

### 2.2.15.3. *Minimal non-isomorphic supergroups*

If $\mathcal{G}$ is a maximal subgroup of a group $\mathcal{S}$, then $\mathcal{S}$ is called a minimal supergroup of $\mathcal{G}$. Minimal non-isomorphic supergroups are again subdivided into two types, the *translationengleiche* or *t* supergroups **I** and the *klassengleiche* or *k* supergroups **II**. For the minimal *t* supergroups **I** of $\mathcal{G}$, the listing contains the index [*i*] of $\mathcal{G}$ in $\mathcal{S}$, the *conventional* Hermann–Mauguin symbol of $\mathcal{S}$ and its space-group number in parentheses.

There are two types of minimal *k* supergroups **II**: supergroups with additional centring translations (which would correspond to the **IIa** type) and supergroups with smaller conventional unit cells than that of $\mathcal{G}$ (type **IIb**). Although the subdivision between **IIa** and **IIb** supergroups is not indicated in the tables, the list of minimal supergroups with additional centring translations (**IIa**) always precedes the list of **IIb** supergroups. The information given is similar to that for the non-isomorphic subgroups **IIb**, *i.e.*, where applicable, the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of $\mathcal{S}$ and its space-group number. The supergroups are listed in order of increasing index and increasing space-group number.

The block of supergroups contains only the *types* of the non-isomorphic minimal supergroups $\mathcal{S}$ of $\mathcal{G}$, *i.e.* each entry may correspond to more than one supergroup $\mathcal{S}$. In fact, the list of minimal supergroups $\mathcal{S}$ of $\mathcal{G}$ should be considered as a backwards reference to those space groups $\mathcal{S}$ for which $\mathcal{G}$ appears as a maximal subgroup. Thus, the relation between $\mathcal{S}$ and $\mathcal{G}$ can be found in the subgroup entries of $\mathcal{S}$.

*Example:* $\mathcal{G}$: $Pna2_1$ (33)

Minimal non-isomorphic supergroups

**I** [2] *Pnna* (52); [2] *Pccn* (56); [2] *Pbcn* (60); [2] *Pnma* (62).

**II** ... [2] $Pnm2_1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmn2_1$, 31); ....

Block **I** lists, among others, the entry [2] *Pnma* (62). Looking up the *subgroup* data of *Pnma* (62), one finds in block **I** the entry [2] $Pn2_1a$ ($Pna2_1$). This shows that the setting of *Pnma* does not correspond to that of $Pna2_1$ but rather to that of $Pn2_1a$. To obtain the supergroup $\mathcal{S}$ referred to the basis of $Pna2_1$, the basis vectors **b** and **c** must be interchanged. This changes *Pnma* to *Pnam*, which is the correct symbol of the supergroup of $Pna2_1$.

*Note on R supergroups of trigonal P space groups:* The trigonal *P* space groups Nos. 143–145, 147, 150, 152, 154, 156, 158, 164 and 165 each have two rhombohedral supergroups of type **II**. They are distinguished by different additional centring translations which correspond to the 'obverse' and 'reverse' settings of a triple hexagonal *R* cell; *cf.* Chapter 1.2. In the supergroup tables of Part 7, these cases are described as [3] *R*3 (obverse) (146); [3] *R*3 (reverse) (146) *etc.*

### 2.2.15.4. *Minimal isomorphic supergroups of lowest index*

No data are listed for isomorphic *supergroups* **IIc** because they can be derived directly from the corresponding data of *subgroups* **IIc** (*cf.* Part 13).

### 2.2.15.5. *Note on basis vectors*

In the *subgroup* data, $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are the basis vectors of the subgroup $\mathcal{H}$ of the space group $\mathcal{G}$. The latter has the basis vectors **a**, **b**, **c**. In the *supergroup* data, $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are the basis vectors of the supergroup $\mathcal{S}$ and **a**, **b**, **c** are again the basis vectors of $\mathcal{G}$. Thus, **a**, **b**, **c** and $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ exchange their roles if one considers the same group–subgroup relation in the subgroup and the supergroup tables.

*Examples*

(1) $\mathcal{G}$: *Pba*2 (32)

Listed under *subgroups* **IIb**, one finds, among other entries, [2] $Pna2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (33); thus, $\mathbf{c}(Pna2_1) = 2\mathbf{c}(Pba2)$.

* For normalizers of space groups, see Section 8.3.6 and Part 15, where also references to automorphisms are given.





references