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The sequence differs somewhat from that in Chapter 2.3 of this volume. In Chapter 2.3, the *klassengleiche* subgroups have been subdivided in more detail according to the different kinds of cell enlargements and the isomorphic subgroups with specific index values have been listed together with the *klassengleiche* subgroups, *i.e.* separately from the infinite series of isomorphic subgroups. A list of the differences in presentation between Chapters 2.3 and 3.2 is given in the Appendix at the end of this volume.

3.1.1.6. *Information for every subgroup*

3.1.1.6.1. *Index*

The entry for every subgroup begins with the index in brackets, for example [2] or [p] or [p^2] (p = prime number).

The index for any of the infinite number of maximal isomorphic subgroups must be either a prime number p, or, in certain cases of tetragonal, trigonal and hexagonal space groups, a square of a prime number p^2; for isomorphic subgroups of cubic space groups the index may only be the cube of a prime number p^3. In many instances only certain prime numbers are allowed (Bertaut & Billiet, 1979; Billiet & Bertaut, 2002; Müller & Brelle, 1995). If restrictions exist, the prime numbers allowed are given under the axes transformations by formulae such as 'p = prime = $3n-1$'.

3.1.1.6.2. *Subgroup symbol*

The index is followed by the Hermann–Mauguin symbol (short symbol) and the space-group number of the subgroup. If a nonconventional setting has been chosen, then the space-group symbol of the conventional setting is also mentioned in the following line after the symbol $\widehat{=}$.

In some cases of nonconventional settings, the space-group symbol does not show uniquely in which manner it deviates from the conventional setting. For example, the nonconventional setting $P22_12$ of the space group $P222_1$ can result from cyclic exchange of the axes, ($\mathbf{b}, \mathbf{c}, \mathbf{a}$) or by interchange of $\mathbf{b}$ with $\mathbf{c}$ ($\mathbf{a}, -\mathbf{c}, \mathbf{b}$). As a consequence, the relations between the Wyckoff positions can be different. In such cases, cyclic exchange has always been chosen.

3.1.1.6.3. *Basis vectors*

The column 'Axes' shows how the basis vectors of the unit cell of a subgroup result from the basis vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ of the space group considered. This information is omitted if there is no change of basis vectors.

A formula such as '$q\mathbf{a}-r\mathbf{b}, r\mathbf{a}+q\mathbf{b}, \mathbf{c}$' together with the restrictions '$p = q^2 + r^2$ = prime = $4n+1$' and '$q = 2n+1 \geq 1$; $r = \pm 2n' \neq 0$' means that for a given index p there exist several subgroups with different lattices depending on the values of the integer parameters q (odd) and r (even) within the limits of the restriction. In this example, the prime number p must be $p \equiv 1$ modulo 4 (*i.e.* 5, 13, 17, ...); if it is, say, $p = 13 = 3^2 + (\pm 2)^2$, the values of q and r may be $q = 3, r = 2$ and $q = 3, r = -2$.[1]

3.1.1.6.4. *Coordinates*

The column 'Coordinates' shows how the atomic coordinates of the subgroups are calculated from the coordinates x, y and z of the starting unit cell. This includes coordinate shifts whenever a shift of the origin is required (*cf.* Section 3.1.3). If the cell of the subgroup is enlarged, the coordinate triplet is followed by a semicolon; then follow fractional numbers in parentheses. This means that in addition to the coordinates given before the semicolon, further coordinates have to be considered; they result from adding the numbers in the parentheses. However, if the subgroup has a centring, the values to be added due to this centring are not mentioned. If no transformation of coordinates is necessary, the entry is omitted.

Example 3.1.1.6.1.

The entry

$$\tfrac{1}{3}x + \tfrac{1}{4}, y + \tfrac{1}{4}, z; \pm(\tfrac{1}{3}, 0, 0)$$

means: starting from the coordinates of, say, 0.63, 0.12, 0.0, sites with the following coordinates result in the subgroup:

0.46, 0.37, 0.0; 0.793333, 0.37, 0.0;
0.1266667, 0.37, 0.0.

Example 3.1.1.6.2.

The entry of an I-centred subgroup

$$\tfrac{1}{2}x, \tfrac{1}{2}y, \tfrac{1}{2}z; +(\tfrac{1}{2}, 0, 0); +(0, \tfrac{1}{2}, 0); +(0, 0, \tfrac{1}{2})$$

means: starting from the coordinates of, say, 0.08, 0.14, 0.20, sites with the following coordinates result in the subgroup:

0.04, 0.07, 0.10; 0.54, 0.07, 0.10;
0.04, 0.57, 0.10; 0.04, 0.07, 0.60;

in addition, there are all coordinates with $+(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$ due to the I-centring:

0.54, 0.57, 0.60; 0.04, 0.57, 0.60;
0.54, 0.07, 0.60; 0.54, 0.57, 0.10.

For the infinite series of isomorphic subgroups, coordinate formulae are, for example, in the form $x, y, \tfrac{1}{p}z; +(0, 0, \tfrac{u}{p})$ with $u = 1, \ldots, p-1$. Then there are p coordinate values running from $x, y, \tfrac{1}{p}z$ to $x, y, \tfrac{1}{p}z + \tfrac{p-1}{p}$.

Example 3.1.1.6.3.

For a subgroup with index $p^2 = 25$ ($p = 5$) the entry

$$\tfrac{1}{p}x, \tfrac{1}{p}y, z; +(\tfrac{u}{p}, \tfrac{v}{p}, 0); u, v = 1, \ldots, p-1$$

means: starting from the coordinates of, say, 0.10, 0.35, 0.0, sites with the following coordinates result in the subgroup:

0.02, 0.07, 0.0; 0.02, 0.27, 0.0; 0.02, 0.47, 0.0;
0.02, 0.67, 0.0; 0.02, 0.87, 0.0;
0.22, 0.07, 0.0; 0.22, 0.27, 0.0; 0.22, 0.47, 0.0;
0.22, 0.67, 0.0; 0.22, 0.87, 0.0;
0.42, 0.07, 0.0; 0.42, 0.27, 0.0; 0.42, 0.47, 0.0;
0.42, 0.67, 0.0; 0.42, 0.87, 0.0;
0.62, 0.07, 0.0; 0.62, 0.27, 0.0; 0.62, 0.47, 0.0;
0.62, 0.67, 0.0; 0.62, 0.87, 0.0;
0.82, 0.07, 0.0; 0.82, 0.27, 0.0; 0.82, 0.47, 0.0;
0.82, 0.67, 0.0; 0.82, 0.87, 0.0.

If Volume A allows two choices for the origin, coordinate transformations for both are listed in separate columns with the headings 'origin 1' and 'origin 2'. If two origin choices are allowed for both the group as well as the subgroup, then it is understood that the origin choices of the group and the subgroup are the same (either origin choice 1 for both groups or origin choice 2 for both). If the space group has only one origin choice, but the subgroup

[1] If the sum of two square numbers is a prime number p, then it is $p = 2$ or $p = 4n+1$, and every prime number of this type can be expressed as such a sum. Index number restrictions of this kind occur among isomorphic subgroups of certain tetragonal space groups. A similar relation occurring among trigonal and hexagonal space groups concerns prime numbers $p = q^2 - qr + r^2$; $p = 3$ or $p = 6n+1$ always holds for integer q, r and every prime number $p = 6n+1$ can be expressed by such a sum. For details, see Müller & Brelle (1995).

references