

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Table 3.3.1.2

Representatives for the sets of lattice symmetry directions in the various crystal families

| Crystal family | Anorthic (triclinic) | Monoclinic | Orthorhombic | Tetragonal | Hexagonal | Cubic |
|------------------------------------|------------------------------|--|---------------------------------------|---------------------------------------|--|---------------------------------------|
| Lattice point group | Schoenflies C_i | C_{2h} | D_{2h} | D_{4h} | D_{6h} D_{3d} | O_h |
| | Hermann–Mauguin $\bar{1}$ | $\frac{2}{m}$ | $\frac{2}{m} \frac{2}{m} \frac{2}{m}$ | $\frac{4}{m} \frac{2}{m} \frac{2}{m}$ | $\frac{6}{m} \frac{2}{m} \frac{2}{m}$ $\frac{3}{m} \frac{2}{m} \frac{2}{m} \dagger$ | $\frac{4}{m} \frac{3}{m} \frac{2}{m}$ |
| Set of lattice symmetry directions | Primary – | [010] <i>b</i> unique [001] <i>c</i> unique | [100] | [001] | [001] | [001] |
| | Secondary – | – | [010] | [100] | [100] | [111] |
| | Tertiary – | – | [001] | [1 $\bar{1}$ 0] | [1 $\bar{1}$ 0] | [1 $\bar{1}$ 0] [110]‡ |

† In this table, the directions refer to the hexagonal description. The use of the primitive rhombohedral cell brings out the relations between cubic and rhombohedral groups: the primary set is represented by [111] and the secondary by [110]. ‡ Only for $43m$ and 432 [for reasons see text].

3.3.1.4.2. Full Hermann–Mauguin symbols

After the classification of the directions of rotation axes, the description of the seven maximal rotation subgroups of the lattice point groups is rather simple. For each representative direction, the rotational symmetry element is symbolized by an integer *n* for an *n*-fold axis, resulting in the symbols of the maximal rotation subgroups 1, 2, 222, 32, 422, 622, 432. The symbol 1 is used for the triclinic case. The complete lattice point group is constructed by multiplying the rotation group by the inversion $\bar{1}$. For the even-fold axes, 2, 4 and 6, this multiplication results in a mirror plane perpendicular to the rotation axis yielding the symbols $(2n)/m$ (*n* = 1, 2, 3). For the odd-fold axes 1 and 3, this product leads to the rotoinversion axes $\bar{1}$ and $\bar{3}$. Thus, for each representative of a set of lattice symmetry directions, the symmetry forms a point group that can be generated by one, or at most two, symmetry operations. The resulting symbols are called *full Hermann–Mauguin (or international) symbols*. For the lattice point groups they are shown in Table 3.3.1.2.

For the description of a point group of a crystal, we use its lattice symmetry directions. For the representative of each set of lattice symmetry directions, the remaining subgroup is symbolized; if only the primary symmetry direction contains symmetry higher than 1, the symbols ‘1’ for the secondary and tertiary set (if present) can be omitted. For the cubic point groups *T* and *T_h*, the representative of the tertiary set would be ‘1’, which is omitted. For the rotoinversion groups $\bar{1}$ and $\bar{3}$, the remaining subgroups can only be 1 and 3. If the supergroup is $(2n)/m$, five different types of subgroups can be derived: *n/m*, $2n$, $\bar{2n}$, *n* and *m*. In the cubic system, for instance, $4/m$, $2/m$, $\bar{4}$, 4 or 2 may occur in the primary set. In this case, the symbol *m* can only occur in the combinations $2/m$ or $4/m$ as can be seen from Table 3.3.1.3.

3.3.1.4.3. Short symbols and generators

If the symbols are not only used for the identification of a group but also for its construction, the symbol must contain a list of generating operations and additional relations, if necessary. Following this aspect, the Hermann–Mauguin symbols can be shortened. The choice of generators is not unique; two proposals were presented by Mauguin (1931). In the first proposal, in almost all cases the generators are the same as those of the Shubnikov symbols. In the second proposal, which, apart from some exceptions (see Section 3.3.4), is used for the international symbols, Mauguin selected a set of generators and thus a list of short symbols in which reflections have priority (Table 3.3.1.3,

column 3). This selection makes the transition from the short point-group symbols to the space-group symbols fairly simple. These short symbols contain two kinds of notation components:

Table 3.3.1.3

Point-group symbols

| Schoenflies | Shubnikov | International Tables, short symbol | International Tables, full symbol |
|----------------------|-------------------------|---|--|
| C_1 | 1 | 1 | 1 |
| C_i | $\bar{2}$ | $\bar{1}$ | $\bar{1}$ |
| C_2 | 2 | 2 | 2 |
| C_s | <i>m</i> | <i>m</i> | <i>m</i> |
| C_{2h} | 2 : <i>m</i> | 2/ <i>m</i> | 2/ <i>m</i> |
| D_2 | 2 : 2 | 222 | 222 |
| C_{2v} | 2 · <i>m</i> | <i>mm</i> 2 | <i>mm</i> 2 |
| D_{2h} | <i>m</i> · 2 : <i>m</i> | <i>mmm</i> | 2/ <i>m</i> 2/ <i>m</i> 2/ <i>m</i> |
| C_4 | 4 | 4 | 4 |
| S_4 | $\bar{4}$ | $\bar{4}$ | $\bar{4}$ |
| C_{4h} | 4 : <i>m</i> | 4/ <i>m</i> | 4/ <i>m</i> |
| D_4 | 4 : 2 | 422 | 422 |
| C_{4v} | 4 · <i>m</i> | 4 <i>mm</i> | 4 <i>mm</i> |
| D_{2d} | $\bar{4}$: 2 | $\bar{4}2m$ or $\bar{4}m2$ | $\bar{4}2m$ or $\bar{4}m2$ |
| D_{4h} | <i>m</i> · 4 : <i>m</i> | 4/ <i>mmm</i> | 4/ <i>m</i> 2/ <i>m</i> 2/ <i>m</i> |
| C_3 | 3 | 3 | 3 |
| C_{3i} | $\bar{6}$ | $\bar{3}$ | $\bar{3}$ |
| D_3 | 3 : 2 | 32 or 321 or 312 | 32 or 321 or 312 |
| C_{3v} | 3 · <i>m</i> | 3 <i>m</i> or 3 <i>m</i> 1 or 31 <i>m</i> | 3 <i>m</i> or 3 <i>m</i> 1 or 31 <i>m</i> |
| D_{3d} | $\bar{6}$ · <i>m</i> | $\bar{3}m$ or $\bar{3}m1$ or $\bar{3}1m$ | $\bar{3}2/m$ or $\bar{3}2/m1$ or $\bar{3}12/m$ |
| C_6 | 6 | 6 | 6 |
| C_{3h} | 3 : <i>m</i> | $\bar{6}$ | $\bar{6}$ |
| C_{6h} | 6 : <i>m</i> | 6/ <i>m</i> | 6/ <i>m</i> |
| D_6 | 6 : 2 | 622 | 622 |
| C_{6v} | 6 · <i>m</i> | 6 <i>mm</i> | 6 <i>mm</i> |
| D_{3h} | <i>m</i> · 3 : <i>m</i> | $\bar{6}m2$ or $\bar{6}2m$ | $\bar{6}m2$ or $\bar{6}2m$ |
| D_{6h} | <i>m</i> · 6 : <i>m</i> | 6/ <i>mmm</i> | 6/ <i>m</i> 2/ <i>m</i> 2/ <i>m</i> |
| <i>T</i> | 3/2 | 23 | 23 |
| <i>T_h</i> | $\bar{6}/2$ | $m\bar{3}$ | 2/ $m\bar{3}$ |
| <i>O</i> | 3/4 | 432 | 432 |
| <i>T_d</i> | 3/ $\bar{4}$ | $\bar{4}3m$ | $\bar{4}3m$ |
| <i>O_h</i> | $\bar{6}/4$ | $m\bar{3}m$ | 4/ <i>m</i> $\bar{3}2/m$ |