

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

lattices, C may be used instead of P , or F instead of I ; cf. Sections 1.5.4 and 2.1.1.2.

- (ii) Readers who have studied Chapter 1.3 may realize that the ‘lattice bases’ defined here are also called ‘primitive bases’ and that both ‘primitive bases’ and ‘conventional bases’ are special cases of bases used in crystallography.

3.1.2. Bravais types of lattices and other classifications

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3.1.2.1. Classifications

By means of the above-mentioned lattice properties, it is possible to classify lattices according to various criteria. Lattices can be subdivided with respect to their topological types of domains, resulting in two classes in two dimensions and five classes in three dimensions. They are called *Voronoi types*. If the classification involves topological and symmetry properties of the domains, 24 *Symmetrische Sorten* (Delaunay, 1933) are obtained in three dimensions and 5 in two dimensions. Other classifications consider either the centring type or the point group of the lattice.

The most important classification takes into account both the lattice point-group symmetry and the centring mode (Bravais, 1866). The resulting classes are called *Bravais types of lattices* or, for short, *Bravais lattices*. Two lattices belong to the same Bravais type if and only if they coincide both in their point-group symmetry and in the centring mode of their conventional cells. The Bravais lattice characterizes the translational subgroup of a space group. The number of Bravais lattices is 1 in one dimension, 5 in two dimensions, 14 in three dimensions and 64 in four dimensions. The Bravais lattices may be derived by topological (Delaunay, 1933) or algebraic procedures (Burckhardt, 1966; Neubüser *et al.*, 1971). It can be shown (Wondratschek *et al.*, 1971) that ‘all Bravais types of the same [crystal] family can be obtained from each other by the process of centring’. As a consequence, different Bravais types of the same crystal family (cf. Section 1.3.4) differ in their centring mode. Thus, the Bravais types may be described by a lower-case letter designating the crystal family and an upper-case letter designating the centring mode. The relations between the point groups of the lattices and the crystal families are shown in Table 3.1.1.1. Since the hexagonal and rhombohedral Bravais types belong to the same crystal family, the rhombohedral lattice is described by hR , h indicating the family and R the centring type. This nomenclature was adopted for the 1969 reprint of *International Tables for X-ray Crystallography* (1952) and for *Structure Reports* since 1975 (cf. Trotter, 1975).

3.1.2.2. Description of Bravais types of lattices

In Fig. 3.1.2.1, conventional cells for the 14 three-dimensional Bravais types of lattices are illustrated.

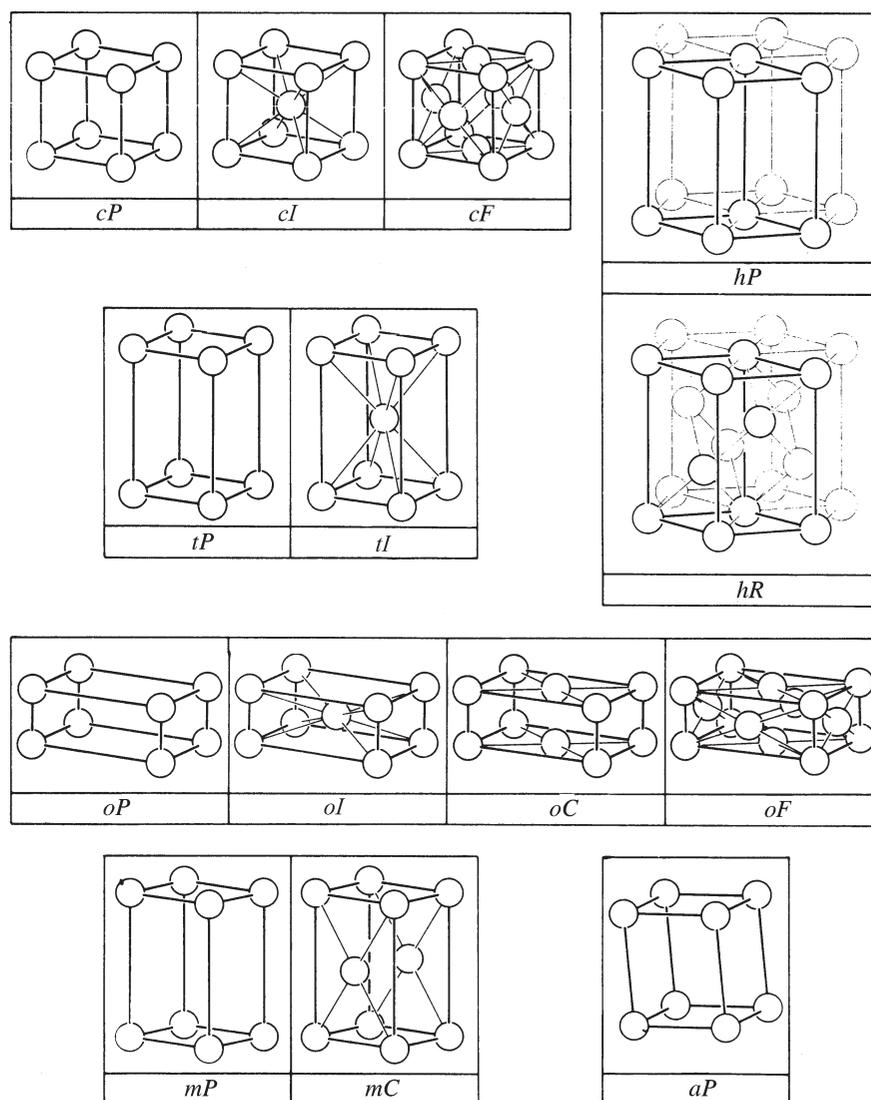


Figure 3.1.2.1

Conventional cells of the three-dimensional Bravais types of lattices (for symbols see Table 3.1.2.2).

In Tables 3.1.2.1 and 3.1.2.2, the two- and three-dimensional Bravais types of lattices are described in detail. For each entry, the tables contain conditions that must be fulfilled by the lattice parameters and the metric tensor. These conditions are given with respect to two different basis systems, first the conventional basis related to symmetry, second a special primitive basis (see below). In columns 2 and 3, basis vectors not required by symmetry to be of the same length are designated by different letters. Columns 4 and 5 contain the metric tensors for the two related bases. Column 6 shows the relations between the components of the two tensors.

The last columns of Tables 3.1.2.1 and 3.1.2.2 show parallel projections of the appropriate conventional unit cells. Among the different possible choices of the primitive basis, as discussed in Section 3.1.1, the special primitive basis mentioned above is obtained according to the following rules:

- (i) For each type of centring, only one transformation matrix P is used to obtain the primitive cell as given in Tables 3.1.2.1 and 3.1.2.2. The transformation obeys equation (3.1.1.2).
- (ii) Among the different possible transformations, those are preferred which result in a metric tensor with simple relations among its components, as defined in Tables 3.1.2.1 and 3.1.2.2.