2.1. Guide to the use of the space-group tables

Th. Hahn, A. Looijenga-Vos, M. I. Aroyo, H. D. Flack, K. Momma and P. Konstantinov

In this part of the volume, tables and diagrams of crystallographic data for the 17 types of plane groups (Chapter 2.2) and the 230 types of space groups (Chapter 2.3) are presented. With the exception of the data for maximal subgroups and minimal supergroups (which have been transferred to Volume A1), the crystallographic data presented in Chapters 2.2 and 2.3 closely follow those in the fifth (2002) edition of Volume A, hereafter *IT* A (2002). This chapter is a guide to understanding and using these data.

Only a minimum of theory is provided here, as the emphasis is on the practical use of the data. For the theoretical background to these data, the reader is referred to Parts 1 and 3, which also include suitable references. A textbook explaining space-group symmetry and the use of the data in Chapters 2.2 and 2.3 (with exercises) is provided by Hahn & Wondratschek (1994); see also Müller (2013).

Section 2.1.1 displays, with the help of an extensive synoptic table, the classification of the 17 plane groups and 230 space groups. This is followed by an explanation of the characterization of the conventional crystallographic coordinate systems, including the symbols for the centring types of lattices and cells. Section 2.1.2 lists the alphanumeric and graphical symbols for symmetry elements and symmetry operations used throughout this volume. The lists are accompanied by notes and cross-references to related IUCr nomenclature reports. Section 2.1.3 explains in a systematic fashion, with many examples and figures, all the entries and diagrams in the order in which they occur in the plane-group and space-group tables of Chapters 2.2 and 2.3. Detailed treatments are given for the Hermann–Mauguin space-group symbols, the space-group diagrams, the general and special positions, the reflections conditions, monoclinic space groups, and the two crystallographic space groups in one dimension (which are also known as the line groups and are treated in Section 2.1.3.16). Section 2.1.4 discusses the computer generation of the space-group tables in this and earlier editions of the volume.

2.1.1. Conventional descriptions of plane and space groups

By Th. Hahn and A. Looijenga-Vos

2.1.1.1. Classification of space groups

In this volume, the plane groups and space groups are classified according to three criteria:

(i) According to *geometric crystal classes*, *i.e.* according to the crystallographic point group to which a particular space group belongs. There are 10 crystal classes in two dimensions and 32 in three dimensions. They are described and listed in Chapter 3.2 and in column 4 of Table 2.1.1.1. [For arithmetic crystal classes, see Chapter 1.3 and Table 2.1.3.3 in this volume, and Chapter 1.4 of *International Tables for Crystallography*, Vol. C (2004).]

(ii) According to *crystal families*. The term crystal family designates the classification of the 17 plane groups into four categories and of the 230 space groups into *six* categories, as displayed in column 1 of Table 2.1.1.1. Here all 'hexagonal', 'trigonal' and 'rhombohedral' space groups are contained in one family, the hexagonal crystal family. The 'crystal family' thus corresponds to the term 'crystal system', as used frequently in the American and Russian literature.

The crystal families are symbolized by the lower-case letters a, m, o, t, h, c, as listed in column 2 of Table 2.1.1.1. If these letters are combined with the appropriate capital letters for the lattice-centring types (*cf.* Table 2.1.1.2), symbols for the 14 Bravais lattices result. These symbols and their occurrence in the crystal families are shown in column 8 of Table 2.1.1.1; mS and oS are the standard setting-independent symbols for the centred monoclinic and the one-face-centred orthorhombic Bravais lattices, *cf.* de Wolff *et al.* (1985); symbols between parentheses represent alternative settings of these Bravais lattices.

(iii) According to *crystal systems*. This classification collects the plane groups into four categories and the space groups into *seven* categories. The classifications according to crystal families and crystal systems are the same for two dimensions.

For three dimensions, this applies to the triclinic, monoclinic, orthorhombic, tetragonal and cubic systems. The only complication exists in the hexagonal crystal family, for which several subdivisions into systems have been proposed in the literature. In this volume [as well as in *International Tables for X-ray Crystallography* (1952), hereafter *IT* (1952), and the subsequent editions of *IT*], the space groups of the hexagonal crystal family are grouped into two 'crystal systems' as follows: all space groups belonging to the five crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$, *i.e.* having 3, 3_1, 3_2 or $\bar{3}$ as principal axis, form the *trigonal* crystal system, irrespective of whether the Bravais lattice is hP or hR; all space groups belonging to the seven crystal classes 6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}2m$ and $6/mmm$, *i.e.* having 6, 6_1, 6_2, 6_3, 6_4, 6_5 or $\bar{6}$ as principal axis, form the *hexagonal* crystal system; here the lattice is always hP (*cf.* Chapter 1.3). The crystal systems, as defined above, are listed in column 3 of Table 2.1.1.1.

A different subdivision of the hexagonal crystal family is in use, mainly in the French literature. It consists of grouping all space groups based on the hexagonal Bravais lattice hP (lattice point symmetry $6/mmm$) into the 'hexagonal' system and all space groups based on the rhombohedral Bravais lattice hR (lattice point symmetry $\bar{3}m$) into the 'rhombohedral' system. In Chapter 1.3, these systems are called 'lattice systems'. They were called 'Bravais systems' in earlier editions of this volume.

The theoretical background for the classification of space groups is provided in Chapter 1.3.

2.1.1.2. Conventional coordinate systems and cells

A plane group or space group usually is described by means of a *crystallographic coordinate system*, consisting of a *crystallographic basis* (basis vectors are lattice vectors) and a *crystallographic origin* (origin at a centre of symmetry or at