Foreword

By Th. Hahn

Symmetry and periodicity are among the most fascinating and characteristic properties of crystals by which they are distinguished from other forms of matter. On the macroscopic level, this symmetry is expressed by point groups, whereas the periodicity is described by translation groups and lattices, and the full structural symmetry of crystals is governed by space groups.

The need for a rigorous treatment of space groups was recognized by crystallographers as early as 1935, when the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* appeared. It was followed in 1952 by Volume I of *International Tables for X-ray Crystallography* and in 1983 by Volume A of *International Tables for Crystallography* (fifth edition 2002). As the depth of experimental and theoretical studies of crystal structures and their properties increased, particularly with regard to comparative crystal chemistry, polymorphism and phase transitions, it became apparent that not only the space group of a given crystal but also its 'descent' and 'ascent', *i.e.* its sub- and supergroups, are of importance and have to be derived and listed.

This had already been done in a small way in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* with the brief inclusion of the *translationengleiche* subgroups of the space groups (see the first volume, pp. 82, 86 and 90). The 1952 edition of *International Tables for X-ray Crystallography* did not contain sub- and supergroups, but in the 1983 edition of *International Tables for Crystallography* the full range of *maximal subgroups* was included (see Volume A, Section 2.2.15): *translationengleiche* (type I) and *klassengleiche* (type II), the latter subdivided into 'decentred' (IIa), 'enlarged unit cell' (IIb) and 'isomorphic' (IIc) subgroups. For types I and IIa, *all* subgroups were listed individually, whereas for IIb only the *subgroup types* and for IIc only the *subgroups of lowest index* were given.

All these data were presented in the form known in 1983, and this involved certain omissions and shortcomings in the presentation, *e.g.* no Wyckoff positions of the subgroups and no conjugacy relations were given. Meanwhile, both the theory of subgroups and its application have made considerable progress, and the present Volume A1 is intended to fill the gaps left in Volume A and present the 'complete story' of the sub- and supergroups of space groups in a comprehensive manner. In particular, *all* maximal subgroups of types I, IIa and IIb are listed individually with the appropriate transformation matrices and origin shifts, whereas for the infinitely many maximal subgroups of type IIc expressions are given which contain the complete characterization of all isomorphic subgroups for any given index.

In addition, the relations of the Wyckoff positions for each group–subgroup pair of space groups are listed for the first time in the tables of Part 3 of this volume.

In the second edition of Volume A1 (2010), additional aspects of group–subgroup relations are included; in particular procedures for the derivation of the minimal supergroups of the space groups are described. Now the minimal supergroups can be calculated from the data for the maximal subgroups to the full extent, with the exception of the low-symmetry (triclinic and monoclinic) space groups. Two new chapters on trees of group–subgroup relations (Bärnighausen trees) and on the Bilbao Crystallographic Server bring these tools closer to the user.

Volume A1 is thus a companion to Volume A, and the editors of both volumes have cooperated closely on problems of symmetry for many years. I wish Volume A1 the same acceptance and success that Volume A has enjoyed.