Scope of this volume

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Group–subgroup relations between space groups, the primary subject of this volume, are an important tool in crystallographic, physical and chemical investigations of solids. These relations are complemented by the corresponding relations between the Wyckoff positions of the group–subgroup pairs.

The basis for these tables was laid by the pioneering papers of Carl Hermann in the late 1920s. Some subgroup data were made available in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), together with a graph displaying the symmetry relations between the crystallographic point groups.

Since then, the vast number of crystal structures determined and improvements in experimental physical methods have directed the interest of crystallographers, physicists and chemists to the problems of structure classification and of phase transitions. Methods of computational mathematics have been developed and applied to the problems of crystallographic group theory, among them to the group–subgroup relations.

When the new series *International Tables for Crystallography* began to appear in 1983, the subgroup data that were then available were included in Volume A. However, these data were incomplete and their description was only that which was available in the late 1970s. This is still the case in the present (fifth) edition of Volume A.

The subgroup data for the space groups are now complete and form the basis of this volume. After introductory chapters on group-theoretical aspects of space groups, on group–subgroup relations and on the underlying mathematical background, this volume provides the reader with:

(1) Complete listings of all maximal non-isomorphic subgroups for each space group, not just by type but individually, including their general positions or their generators, their conjugacy relations and transformations to their conventional settings.

(2) Listings of the maximal isomorphic subgroups with index 2, 3 or 4 individually in the same way as for non-isomorphic subgroups.

(3) Listings of all maximal isomorphic subgroups as members of infinite series, but with the same information as for the non-isomorphic subgroups.

(4) The listings of Volume A for the non-isomorphic supergroups for all space groups.

(5) Two kinds of graphs for all space groups displaying their types of *translationengleiche* subgroups and their types of non-isomorphic *klassengleiche* subgroups.

(6) Listings of all the Wyckoff positions for each space group with their splittings and/or site-symmetry reductions if the symmetry is reduced to that of a maximal subgroup. These data include the corresponding coordinate transformations such that the coordinates in the subgroup can be obtained directly from the coordinates in the original space group.

In this second edition all misprints and errors found up to now have been corrected and the number of illustrating examples has been increased.

In addition, a few changes and extensions have been introduced to facilitate the use of the volume and to extend its range:

(7) The subgroup tables, in particular those of the isomorphic subgroups, have been homogenized.

(8) The data for the minimal supergroups are sufficient to derive all minimal supergroups starting from the subgroup data, with the exception of the *translationengleiche* supergroups of triclinic and monoclinic space groups. The procedures by which this derivation can be achieved are described in detail. The supergroup data are useful for the prediction of high-temperature phase transitions, including the search for new ferroelectric and/or ferroelastic materials, for the treatment of the problem of overlooked symmetry in structure determination and for the study of phase transitions in which a hypothetical parent phase plays an important role.

(9) A new chapter is devoted to the construction of family trees connecting crystal structures (Bärnighausen trees). In a Bärnighausen tree the relations between the Wyckoff positions occupied in the different crystal structures are accompanied by the relations between the corresponding group–subgroup pairs of space groups. Such trees display the additional degrees of freedom for the structural parameters of the low-symmetry phases:

   (*a*) the possibility of distortions due to reduction of site symmetries;

   (*b*) chemical variations (atomic substitutions) allowed for atomic positions that have become symmetry-independent.

   Bärnighausen trees visualize in a compact manner the structural relations between different polymorphic modifications involved in a phase transition and enable the comparison of crystal structures and their classification into crystal-structure types.

(10) A new chapter is dedicated to the Bilbao Crystallographic Server, http://www.cryst.ehu.es/. The server offers freely accessible crystallographic databases and computer programs, in particular those related to the contents of this volume. The available computer tools permit the studies of general group–subgroup relations between space groups and the corresponding Wyckoff positions.

The data in this volume are indispensable for a thorough analysis of phase transitions that do not involve drastic structural changes: the group–subgroup relations indicate the possible symmetry breaks that can occur during a phase transition and are essential for determining the symmetry of the driving mechanism and the related symmetry of the resulting phase. The group–subgroup graphs describing the symmetry breaks provide information on the possible symmetry modes taking part in the transition and allow a detailed analysis of domain structures and twins.