Scope of this volume

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Group–subgroup relations between space groups, the subject of this volume, are an important tool in crystallographic, physical and chemical investigations. In addition to listing these relations, the corresponding relations between the Wyckoff positions of the group–subgroup pairs are also listed here.

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 and 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, group–subgroup relations between space groups and the underlying mathematical background, this volume provides the reader (in many cases for the first time) 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 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 non-isomorphic subgroups;

(4) data for non-isomorphic supergroups for all space groups (these are already in Volume A) such that the subgroup data may be reversed for problems that involve supergroups of 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 the splittings of all Wyckoff positions for each space group if its symmetry is reduced to that of a subgroup. These data include the corresponding coordinate transformations such that the coordinates in the subgroup can be obtained easily from the coordinates in the original space group;

(7) examples explaining how the data in this volume can be used.

The subgroup 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 they 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. The subgroup relations between the space groups also determine the possible symmetries of intermediate phases that may be involved in the transition pathway in reconstructive phase transitions.

The data in this volume are invaluable for the construction of graphs of group–subgroup relations which visualize in a compact manner the relations between different polymorphic modifications involved in phase transitions and which allow the comparison of crystal structures and their classification into crystal-structure types. Particularly transparent graphs are the family trees that relate crystal structures in the manner developed by Bärnighausen (1980) (also called Bärnighausen trees), which also take into account the relations of the Wyckoff positions of the crystal structures considered. Such family trees display the additional degrees of freedom for the structural parameters of the low-symmetry phases, the possibilities of adapting to different kinds of distortions by reduction of site symmetries and the chemical variations (atomic substitutions) allowed for atomic positions that have become symmetry-independent.

The data on supergroups of space groups 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.