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Structure Types

Part 3

Space groups (194) $P6_3/mmc$ – (190) $P-62c$

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Preface

In the 1970s Landolt-Börnstein published a series of volumes containing crystallographic data for organic (III/5 Structure Data of Organic Crystals), intermetallic (III/6 Structure Data of Elements and Intermetallic phases) and inorganic compounds (III/7 Crystal Structure Data of Inorganic Compounds). During the 30 years that have passed, the experimental methods leading to a complete structure determination have considerably improved and the large number of crystal structures known today justifies the publication of a new compilation.

The present volume will cover both intermetallic and classical inorganic compounds, a clear limit having been drawn by excluding compounds that contain C-H bonds. Whereas the earlier edition listed space group/crystal system and cell parameters for different classes of compounds, we have here chosen a different approach by grouping known crystal structures into structure types. The structure type concept is widely used among inorganic compounds, where the number of isotypic compounds can reach several hundreds. The first subvolumes will contain complete crystallographic data sets, including atom coordinates, that represent distinct structure types, whereas the last subvolumes will list cell parameters of isotypic compounds. The crystallographic data are accompanied by remarks and crystallographic features common to isotypic compounds, such as the atomic environments, a brief description of the main structural features, and drawings of selected structure types.

In the definition used here, structures belonging to the same structure type crystallize in the same space group, have similar cell parameters and similar representative atom coordinates. The latter criterion requires that they are isopointal, i.e. they have the same Wyckoff sequence (sequence of Wyckoff positions). Following this scheme, the structure types are ordered according to the space group number and the Wyckoff sequence. The present subvolume, the third of the series, contains data for some 700 hexagonal (space groups # 194 to 190) structure types, reported up to the year 2003.

We would like to thank the coauthors for their contribution and all other collaborators on the databases TYPIX and Pauling File, who have, through the years, helped in compiling and analyzing the large number of structural data that constitute the basis of this work.

Switzerland, July 2005

The Editors

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