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Group theory applied to chemistry. (English) Zbl 1304.92008

Theoretical Chemistry and Computational Modelling. Dordrecht: Springer (ISBN 978-94-007-6862-8/hbk; 978-94-007-6863-5/ebook). xiii, 269 p. (2013).

As the author explains in the preface, the purpose of this text is to "relate our macroscopic intuitive ideas about symmetry to the molecular world." The material in the book is organized into seven chapters. In Chapter 1, the precise meaning of the statement that a symmetry operation acts on a point in the space, on a function, and on an operator is examined and the difference between active and passive views of symmetry is explained. Basic facts on function spaces, linear operators and matrices are collected in Chapter 2. The concept of a group is introduced in Chapter 3 with the example of a symmetry group of the ammonia molecule. An overview of molecular symmetry groups is given and the relationship between rotational groups and chirality is explained.

Chapter 4 deals with the fundamental notion of irreducible representations and related topics. The character theorem, matrix theorems, and projection operators are introduced here. A detailed group-theoretical analysis of three chemical applications, the tetrahedral hybridization of carbon, the molecular vibrations of UF_6, and the electronic structure of conjugated hydrocarbons is offered. The relationship between irreducible representations and quantum chemistry is addressed in Chapter 5. Starting with a brief introduction to the prequantum principles of symmetry, the author proceeds by analyzing the concept of degeneracy. It is shown how the degenerate components can be characterized by canonical symmetry relationships. Finally, symmetry operations that leave the Hamiltonian invariant are discussed.

Chapter 6 deals with interactions expressed as matrix elements of operators in a function space. The Wigner-Eckart theorem is introduced here together with the symmetry selection rules. The results are applied then to chemical reaction theory and to the theory of the Jahn-Teller effect. In the concluding part, the polyhedral Euler theorem is introduced and applied to valence-bond theory for clusters. Spherical symmetry and spins are discussed in Chapter 7, where applications in crystal-field theory and electron spin resonance are also considered. Useful information including character tables, facts on spherical, binary and cylindrical groups, subduction and induction, direct-product tables is collected in Appendices A–G. In the end of the book, the reader will find solutions to problems, references and an index.

In the preface to the book, the author promises that "[i]n the end the reader should have acquired the skills to make use of the mathematical tools of group theory for whatever chemical problem he/she will be confronted with the course of his or her own research." Certainly, the text serves its purpose; it provides a valuable source of information for motivated graduate students and researchers interested in applications of group theory in chemistry.

Reviewer: Yuriy V. Rogovchenko (Kristiansand)

MSC:

92-02 Research exposition (monographs, survey articles) pertaining to biology
92E10 Molecular structure (graph-theoretic methods, methods of differential topology, etc.)
20H15 Other geometric groups, including crystallographic groups

Keywords:

chemistry; symmetry; group theory; representations; interactions

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