Theor Chim Acta (1992) 82: 339–340

Theoretica Chimica Acta

Book reviews

Fujita, S. 1990: Symmetry and combinatorial enumeration in chemistry. Springer-Verlag, New York Berlin Heidelberg, ix + 368 pp. (ISBN 0-387-54126-8) $39.00

In a number of recent articles in several journals (including Theoretica Chimica Acta), Dr. Fujita has developed powerful new group-theoretical techniques for the treatment of problems such as symmetry classification of molecules and isomer enumeration. The present book brings these techniques together in one place, presenting them in a unified manner, and is thus most welcome.

Although the book is in principle self-contained, containing some introductory chapters on the fundamentals of group theory, it would be quite difficult going for a novice and is not recommended as an introduction to group theory. On the other hand, a reader who already understands basic ideas of group theory, and who is willing to think mathematically, may find the study of this book most rewarding.

Basic to Fujita's approach are two related concepts which are not really new, but which are not discussed in other books on group theory addressed to chemists. These are the concepts of coset representation and table of marks. Although these concepts may seem strange at first, they are really no more difficult than more familiar concepts such as that of irreducible representation. Given a group G and a subgroup G_i, each element of G applied to a coset of G_i gives another coset, and thus each element of G can be thought of as a permutation of the cosets, leading to a representation of G in terms of such permutations, called the coset representation $G(/G_i)$. Given two subgroups G_i and G_j of G, the mark m_{ij} of G_j on $G(/G_i)$ is defined as the number of cosets of G_i left invariant by G_j. It is fairly easy to prove that $m_{ij} = 0$ unless G_j, or a subgroup conjugate to it, is a subgroup of G_i. For example, if G_i is the subgroup leaving a particular site invariant, each coset corresponds to a site equivalent to the original one, and $G(/G_i)$ is the representation of G in which each element is pictured as permuting these equivalent sites. A subgroup G_j of G_i may leave more than one of these equivalent sites invariant, and the number that it leaves invariant is by definition m_{ij}.

With the aid of these concepts, Fujita develops a method for the systematic classification of molecular symmetry and chirality types in terms not only of the point group of the molecule, but of "orbits" (sets of equivalent sites) and the subgroups leaving sites of each orbit invariant.

A typical isomer enumeration problem is the following: For a given skeleton with n sites and skeletal symmetry group G, and a given assortment of ligands, how many isomers are there with symmetry G_j, where G_j is an arbitrary subgroup of G? With the aid of mark tables and the concept of coset representation, Fujita shows how to solve this type of problem for various situations, including the case where the ligands are allowed to have internal structure (chiral or rotating ligands) and the case where some of the sites (e.g., bridge sites) can be occupied only by ligands of a certain minimum valence.

Essential to Fujita's approach is the availability of mark tables for the various molecular point groups. Typically, the mark table of a group is somewhat easier to construct than its character table, once one gets the hang of it, but as in the case of character tables it is often nice to have the tables provided. The present book has appendices with mark tables of the most important molecular point groups, and other tables related to these that are useful in applying the techniques developed in the book.

This book is not easy going, but the reader who makes the necessary effort will not regret it. Mark tables have the potential of being approximately as useful to chemists as character tables; if the coming generation of chemists learn to appreciate this fact, it will probably be due in large part to the influence of this book.

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Chemical graph theory, introduction and fundamentals.
Edited by D. Bonchev and D. H. Rouvray

This book consists of six chapters, each written by a different expert in chemical graph theory, an area which may be reviewed to provide the natural mathematical framework for the quantitative codification of classical molecular-structure and chemical-bonding ideas. Throughout most of the book atoms correspond to vertices of a graph while chemical bonds correspond to graph edges. The first chapter by D. H. Rouvray is a nice historical survey of molecular valence structures as graphs, with the story stopping short of modern quantum-chemical results of the last few decades. The second chapter by the late O. E. Polansky is a concise readable account of much formal graph theory relevant for chemistry. The third chapter by A. L. Goodson concerns organic molecular nomenclature from its beginnings up through modern graph-theoretically framed ideas, where for instance, one seeks a "canonical" labelling for the vertices of a graph. The fourth chapter by I. Gutman describes a selection of graph-theoretic polynomials, each being a generating function for a "graded" class of subgraphs of the parent (molecular) graph. The fifth chapter by A. T. Balaban is a thorough discussion of the isomer enumeration problem with some overlap into the theory of degenerate rearrangements and reaction graphs. The last chapter by N. Trinajstić is a rather brief summary of a graph-theoretic approach to Hückel molecular-orbital theory. Throughout the book the emphasis is less on detailed proofs and more on the presentation of ideas, theorematic statements, and illustrative examples.

Overall the book is quite understandable, and offers a survey of a reasonable fraction of chemical graph theory. Other aspects of chemical graph theory concern: its use in structure-activity relations, its connection with perturbation theory via Feynman diagrams, its utility in analyzing kinetic responses in dynamical systems, its occurrence in key polymer statistics problems or a variety of other many-body statistical-mechanical models, its relevance in modern valence-bond theory, its use in representing group actions (as in "GUGA"), etc. Evidently, such are conceivable topics for a second volume on chemical graph theory in the "Mathematical Chemistry Series" of which this book is the first member.

There is some part of an answer to a question raised in a recent review in this journal (79:433). There W. Kutzelnigg asks "Will Mathematical Chemistry remain centered around Hückel theory, and molecular topology?" Evidently from the discussion of the preceding paragraphs only a fraction of even the restricted area of chemical graph theory is focused on Hückel theory. Further the future volumes in this "Mathematical Chemistry Series" edited by Bonchev and Rouvray are planned to include consideration of artificial intelligence, combinatorics, group theory, information theory, linear algebra, and topology.

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