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Book review

King, R. B., Rouvray, D. H.: Graph theory and topology in chemistry. Elsevier, Amsterdam New York 1987 (ISBN 0-444-42882 (Vol 51) and 0-444-41699-4 (Series)) $183

This volume is no. 51 in the series *Studies in physical and theoretical chemistry* and it represents the proceedings of an international conference held on March 16-20, 1987, at the University of Georgia in Athens, Georgia, USA, on the subject indicated in the title. The articles are photo-reproduced from the individual typescripts.

The subject matter is subdivided into five sections, namely
A. Knot theory and reaction topology;
B. molecular complexity, system similarity, topological indices;
C. polyhedra clusters and the solid state;
D. eigenvalues, conjugated systems, resonance;
E. coding, enumeration, data reduction.

Section A contains articles on the relation between knot theory and biological macromolecules, chemical reactions and topological stereo-chemistry. Other subjects are a topological approach to the stereochemistry of non-rigid molecules, the chirality of Möbius ladders, topological chirality indices, and the topology of energy surfaces. It concludes with discussions on network thermodynamics and kinetics, its fundamental covariant aspects and its relevance to the chemistry for living systems.

Section B begins with basic discussions of the criteria for measures of topological complexity and of topological indices and graph invariants. Several articles deal with the physicochemical properties of alkanes and topological indices. The use of the fractal concept and of Wiener numbers is given special attention. The concluding articles deal with quantitative molecular similarity analysis in large biomedical compounds by a variety of topological descriptors including subgraph isomorphisms, maximum common structures, molecular similarity and dissimilarity indices and others.

Section C starts with several articles in which chemical reaction network graphs are used to elucidate interconversions of isomers in octacoordinate square antiprisms, in axially distorted octahedra, and in closo-carboranes. A lucid presentation on the essential role of topology rather than symmetry for the successful variants of the generalized Hückel approach contains a range of applications to organic chemistry, to transition metal complexes, to various types of symmetry distortions, to the Woodward Hoffman rules and to solids. It is followed by a discussion of metal clusters and superconductors from a topological viewpoint. The final articles deal with the use of topological lattices for stochastic problems, in particular the statistical thermodynamics of phase transitions in metal clusters, the use of random graphs for polymerization models and the generation of random graphs for physical systems.

The material in Section D is mostly concerned with the kind of topological graphs associated with π-electron theory. The first two contributions provide new approaches towards the determination of spin multiplicities in multiradical molecules, in networks and in organic ferromagnets. A simple bond orbital resonance theory is described. Several articles deal with the simple determination of resonance energies in complex and large systems, in particular by the conjugated circuit theory and by the transfer matrix approach. The eigenvalue determination in heterocycles by means of functional partial

graphs is discussed. An examination of the properties of Kekulé structures and sextett patterns concludes this section.

Three contributions in Section E deal with the encoding and enumeration of benzenoid graphs, by an initial examination of the perimeter, by factorization and specifically for rectangular perimeters. Other articles discuss the counting of isomers and isomerizations by Redfield enumeration and the transfer of graph-tree counting from a plane to the surface of a sphere as might be appropriate for the recently discussed balloon-type molecules. Two articles outline a broader view of the chemical applications of computational graph theory and of the reduction of information with the help of graphs.

This book is valuable in that it provides a broad survey over the many different areas of chemistry in which graph theoretical and topological techniques are currently providing insight and stimulation. The book is probably of greatest interest to the professionals in this field as a mirror of the state of the art. For those outsiders who are appreciative of the fundamental fact that the connectivity between atoms lies at the very heart of chemistry, on the other hand, the book can serve as a useful compilation of some of the best of current thinking on these matters. The decision whether to buy the book or not will however also be influenced by the hefty price tag.

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