PRIKAZI KNJIGA BOOK REVIEWS

A. T. Balaban (Editor)
From Chemical Topology to Three-Dimensional Geometry

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This book appeared in the series »*Topics in Applied Chemistry*«, which is edited by Professor Alan R. Katritzky, FRS (University of Florida, Gainesville, USA) and Dr Gebran J. Sabongi (Encapsulation Technology Center, 3-M, St. Paul, Minnesota, USA) and published by Plenum Press of New York. »*From Chemical Topology to Three-Dimensional Geometry*«, edited by the well-known organic and mathematical chemist Professor Alexandru T. Balaban (Polytechnic University, Bucharest, Romania), consists of the Preface (3 pages) and 10 chapters. Each chapter was written by an author or authors who are leaders in the field of chemical applications of discrete mathematics and who have personally contributed to the recent exciting development of mathematical chemistry. They produced an up-to-date account of mathematical and computational methods for representing molecular systems in the 3D world and their use for designing molecules and predicting molecular properties.

The first chapter (24 pages), entitled »*From Chemical Graphs to 3D Molecular Modeling*«, was written by the editor, Alexandru T. Balaban. In this chapter, the author describes methods for obtaining the numerical representation of molecules in 2D and 3D spaces. The second chapter (18 pages) is entitled »*Descriptors of Molecular Shape in 3D*« and was written by Paul G. Mezey (Department of Chemistry and Department of Mathematics and Statistics, University of Saskatchewan, Saskatoon, Canada). This is an important chapter because the molecular shape is a fundamental structural characteristic for understanding static and dynamic properties of molecules. In this chapter, the author describes his original method for predicting the shapes of various molecules, including macromolecules. The third chapter (29 pages), entitled »*3D Molecular Design – Searching for Active Conformers in QSAR*,« was written by Ovanes G. Mekenyan (Department of Physical Chemistry, Bourgas University, Bourgas, Bulgaria and Lake Superior Research Institute, University of Wisconsin-Superior, Superior, Wisconsin, USA) and Gilman D. Veith (National Health and Environmental Effects Research Laboratory, U.S.E.P.A., Research Triangle Park, N.C., USA). The authors describe the basic concepts of applying 3D chemical models to the

design of new compounds that have sought-after properties. The acronym QSAR stands for the quantitative structure-activity relationships. The fourth chapter (44 pages) is entitled »*Use of Graph-Theoretic and Geometrical Molecular Descriptors in Structure-Activity Relationships*« and was written by Subhash C. Basak, Gregory D. Grunwald and Gerald J. Niemi (Center for Water and the Environment, Natural Resources Research Institute, University of Minnesota, Duluth, Minnesota, USA). This is an application-oriented chapter. The authors reviewed the 2D and 3D topological indices and their application in QSAR. The fifth chapter (42 pages), entitled »*Recognition of Membrane Protein Structure from Amino Acid Sequence*«, was written by Bono Lučić, Nenad Trinajstić (The Rugjer Bošković Institute, Zagreb, Croatia), and Davor Juretić (Department of Physics, Faculty of Science, Split, Croatia). In this chapter, the authors present their method for predicting the membrane protein structures from the constituting amino acids. The sixth chapter (78 pages) is entitled »*On Characterization of 3D Molecular Structure*« and was written by Milan Randić (Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa, USA) and the late Marko Razinger (National Institute of Chemistry, Ljubljana Slovenia). In this chapter, rather lengthy and rich in ideas, the authors discuss the nature of the chemical structure, the 3D representation of molecules by means of molecular and shape profiles and their application in QSPR (quantitative structure-property relationships).

Apparently, no modern chemical text can appear without mentioning fullerenes, a fascinating class of all-carbon cage molecules. In this book, there are three chapters on fullerenes and related structures. The seventh chapter (26 pages), entitled »*Chemical Graph Theory of Fullerenes*,« and was written by Patrick W. Fowler (Department of Chemistry, University of Exeter, Exeter, England). This chapter contains answers to the following questions: What is fullerene? and How many fullerenes are there? It also discusses the electronic structure, stability and reactivity of fullerenes. The eighth chapter (34 pages) is entitled »*Recent Work on Toroidal and Other Exotic Fullerene Structures*« and was written by Edward C. Kirby (Resource Use Institute, Pitlochry, Perthshire, Scotland). In this chapter, the author discusses toroidal fullerenes and their properties and stabilities. The ninth chapter (45 pages), entitled »*All-Conjugated Carbon Species*,« was written by Douglas J. Klein and Hongyao Zhu (Department of Marine Sciences, Texas A&M University, Galveston, Texas, USA). This chapter contains procedures for constructing all kinds of carbon systems, including fullerenes. The final, tenth chapter (72 pages) is entitled »*Applications of Topology and Graph Theory in Understanding Inorganic Molecules*« and was written by R. Bruce King (Department of Chemistry, University of Georgia, Athens, Georgia, USA). This lengthy chapter presents the energetics and stabilities of inorganic cages and clusters.

»*From Chemical Topology to Three-Dimensional Geometry*« will be useful to graduate students and research scientists of various profiles, such as

chemists, biochemists, medicinal chemists, mathematical chemists, applied mathematicians, statisticians, chemical biologists, drug designers, *etc.* The reason for this is simple: the authors tried to describe what modern mathematical chemistry can offer in (bio)molecular modeling, in fullerene research and drug design. Futhermore, the authors have also set the path for the development of mathematical chemistry to the end of this century and even in the first decade of the 21st century. This links well with the recent statement by Alan Katritzky, Mati Karelson and Victor S. Lobanov (*Pure Appl. Chem.* **69** (1997) 245–248): »As scientists, today we are increasingly urged to do science of relevance to society. QSPR allows us to carry out science that will undoubtedly help us to make the production of new molecules useful in all faces of life and society more cheaply, more efficiently, and in a more environmentally friendly manner. At the same time, it offers the highest intellectual challenges for the development of meaningful relationships, novel theories, and deepest understanding into the molecular nature of the world in which we live.«

Nenad Trinajstić