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Modern Conformational Analysis

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xii + 264 pages, 703 references.
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The development of chemistry, especially of computer chemistry, is so overhelming that it is virtually impossible to grasp all the developments simply by reading original scientific papers and even by reading review articles. Therefore, books that deal with wide topics are more than ever needed. This is one of such books and is aimed at – as the author states in the preface – »organic and physical chemists who are acquainted with classical conformational analysis and want to learn more about recent developments and perspectives in this field«. These recent developments are not, however, new methods but »novel exciting molecular structures« and approaches, namely computer-assisted molecular design (CAMD) which is based on extensive use of all kinds of theoretical methods for explanation and forecasting of experimantal results.

The book is divided in 12 chapters. In the Introduction, the author gives the basic stereochemical ideas (conformation, isomerism, stereoisomerism *etc.*) and the applications of these ideas: one-pot chemical synthesis, self-assembly of RNA-viruses, synthesis of molecules of unusual structure (cubane, fullerene, coronane), supramolecular complexes with cyclodextrins, crown ethers *etc.* The next chapter is devoted to physical methods that have been used in conformational analysis: diffraction methods (X-ray, neutron diffraction, electron diffraction), spectroscopic methods (microwave, IR, Raman, UV, CD, and NMR spectroscopy), and to quite novel methods based on scanning probe microscopy (STM and AFM). The reader will not learn much about the principles of these methods, but should find very useful examples of their application in conformational analysis and interesting references. In the third chapter, theoretical methods (quantum chemistry, molecular mechanics, molecular dynamics, Monte Carlo) and essentials of statistical mechanics are described. The reader surely could not comprehend such a wide variety of topics by reading a few (altogether 22) pages, especially when the

author wants to go into the details (she used near a whole page to explain the wave functions for hydrogen atom, which is irrelevant for the application of quantum mechanics to molecules), and this is – in my opinion – the worst part of the book.

The next two chapters are devoted to molecular symmetry (Ch. 4) and chirality (Ch. 5). These chapters are really »modern«: the symmetry is explained on molecules of quite unusual structure, and the Cahn-Ingold-Prelog R/S system is discussed and criticized giving the new approaches to define the chiral molecules. In spite of their brevity (15 pages), the author has succeeded in mentioning such a peculiarity like the presence of D-amino acids in the living organisms, geological dating using the rate of racemization reaction and novel theories of the origin of monochirality during bioneogenesis.

The other half of the book is devoted to the application of conformational analysis to scpecific molecular systems. After a short overview of standard structures of organic molecules (Ch. 6), the author describes unusual saturated (Ch. 7) and unsaturated molecules (Ch. 8). The »planar methane problem« and pyramidal carbon atoms are throughfully discussed along with nonstandard multiple bonds. Structures with very distorted coordination polyhedrons, like those of fenestranes, hexaprismane (planar cyclohexane ring!), triprismane, cyclic cumulenes, nonlinear alkynes and cyclophanes, are presented, together with very instructive stories about their synthesis and theoretical background for their existence. Two pages and 15 references are devoted to fullerenes.

The ninth chapter deals with molecules of unusual topology (dendrimers, catenanes, molecules mimicking Möbius strip, mesoionic compounds) and the tenth chapter is devoted to self-assembling objects, *i.e.* supramolecular structures. Very interesting is the paragraph which deals with cyclodextrins, their structure, conformational flexibility and applications in preparative chemistry (chromatographic separation of diastereomers and enantiomers), pharmacology (microencapsulation of drugs) and photoelectronics. Formation of mono- and polylayers, micelles, vesicles and Langmuir-Blodgett films is also described and the chemical reactions (cascade cyclization, »zipper reactions«) based on self-assembly of molecules are presented.

After a short introduction on molecular modeling (Ch. 11), with mention of most frequently used programmes for conformational analysis and application of QSAR in drug design, the last chapter deals with the present and future applications of conformational analysis. Exciting is the story of molecules designed for future applications in molecular electronics (chemionics), which almost resembles science fiction: molecular wires, ionic transmitters and detectors, organic metals and organic switches (bistabils).

At the end, it can be said that the value of the book is not so much in the presentation of methods but in the presentation of the application of conformational analysis (or, to use a more modern term, molecular modeling)

in the design of novel compounds of unusual structure (more than 360 structures are presented in the book!). The book is unfortunately limited only to the conformational analysis of organic compounds (in spite of the growing literature on coordination and organometallic compounds in recent times), but it is dubious whether it would be possible to present such a wide topic briefly.

The book will be of interest to graduate students in chemistry (expecially to those specializing in structural and organic chemistry); however, it is worth reading to any chemist interested in modern structural chemistry.