CROATICA CHEMICA ACTA
CCACAA **80** (2) A23–A24 (2007)

BOOK REVIEWS

Mircea V. Diudea, Margareta S. Florescu, and Padmakar V. Khadikar

Molecular Topology and Its Applications

EfiCon Press, Bucharest, 2006, VI+382 pp.,
ISBN (10) 973-87904-0-9;
ISBN (13) 978-973-87904-0-7

The book describes a large class of molecular-graph-based structure descriptors (»topological indices«) and a large number of their chemical applications. As the authors say, their primary aim was »*writing this book to present Topology as it is today*« and »*to make chemists familiar with the fascinating mathematical theory as well as make mathematicians understand chemical applications of Graph Theory*«. Under »topology« (both in the title of the book and in this quotation) are understood those aspects of molecular structure which can be represented by means of molecular graphs. The book is mainly concerned with matrices and matrix invariants associated with molecular graphs, and their chemical applications.

The book consists of the preface, nine chapters and eleven appendices. Each chapter is followed by a long list of references.

In Chapter 1, the elements of graph theory are briefly outlined (on only 9 pages). Thus, a reader who has no previous knowledge in this area had better consult a more extensive source.

Chapter 2 presents the numerous matrices by which »molecular topology« can be described. Definition, together with an illustrative example, is given for each of these matrices. The basic mathematical properties of the matrices are also mentioned.

Chapter 3 is a survey of some (but certainly not all) molecular-structure descriptors that can be obtained from the matrices described in Chapter 2. Again, the definition is provided for each of these descriptors, with in many cases the respective calculation illustrated by pertinent examples. The basic mathematical properties of these indices, as well as many of the known relations between them, are also found in Chapter 3.

The considerations from Chapter 3 are continued in Chapter 4, in which a specific group of structure-descriptors are studied in due detail. These are the classical Wiener index and several of its more recently proposed variants. In the language of graph theory, Chapter 4 deals with chemically relevant distance-based graph invariants.

In Chapter 5, the authors make an excursion to the somewhat unrelated topics of molecular symmetry and similarity. Evidently, this was done because one author (Diudea) did a lot of work in this area.

Chapter 6 is an »outlier« as well. It presents the main notions and methods of statistics, needed for the construction of *QSPR* and *QSAR* models. Recall that *QSPR* = **Q**uantitative **S**tructure-**P**roperty **R**elation, *QSAR* = **Q**uantitative **S**tructure-**A**ctivity **R**elation, with »property« meaning a certain quantity encountered in physical chemistry, whereas »activity« refers to some quantity relevant to the biological, pharmacological, environmental, or similar role of the compound considered. Recall also that *QSPR* and *QSAR* models provide the main chemical applications of the molecular-graph-based structure-descriptors. Chapter 6 is written in a concise, clear, and precise manner, so that – in the opinion of the reviewer – this part of the book could become a preferred starter to those who want to perform and to understand *QSPR* and *QSAR* studies.

Chapter 7 returns to the main topic of the book. In it, the theory of the Szeged index is outlined in detail, and then its countless applications are listed. It should be noted that the Szeged index is also a distance-based graph invariant, closely related to the Wiener index. This chapter contains almost everything that one author (Khadikar) did (and published) in connection with the Szeged index. Applications of the Szeged index in physical, medicinal, and environmental chemistry, pharmacology, and toxicology are remarkably numerous. As examples, we mention the modeling of polychlorinated biphenyls in the environment, of proton-ligand formation constants, of hydrophobicity of polyacenes, of NMR chemical shifts, of CH-acidity, of steric strain, of antituberculotic activity of quinolones, of anti-inflammatory activity of phenols, of receptor binding potency of indolealkylamine, of toxicity of nitrobenzenes, *etc. etc*.

Chapter 8 outlines the theory and applications of a close relative of the Szeged index – the *PI* index. After a very detailed survey of the methods for calculating the *PI* index, we learn about its applications, such as for prediction of the lipophilicity of alkanes, cycloalkanes, and polychlorinated biphenyls, of inhibition potential of benzoyl alcohols against certain fungi, *etc.*

Chapter 9 entitled »*Exhaustive Information*« embraces also the eleven Appendices. In this reviewer's opinion, the word »exhaustive« is not justified; the published material in chemical graph theory is so abundant, and the development of this area so rapid, that nowadays no collection of information should and could be considered as »exhaustive«. Anyway, Chapter 9 provides a list of main chemical applications of the topological indices, with pertinent references to the sources. The first nine Appendices contain lists of various structure-descriptors (especially those mentioned in the book), with their symbols indicated. Appendix 10 is a collection of references relating to prediction of physicochemical properties, biological activity, and toxicity, while Appendix 11 contains similar data on *QSPR* and *QSAR* models.

Each part of the book is richly illustrated with figures, diagrams, and tables, so that the text is a pleasure to read and chemists can easily follow and understand it.

The book will be useful to all those who are interested in molecular-graph-based structure descriptors and, especially, in their applications. It will be particularly useful to chemistry students (undergraduate and graduate) who want to learn the elements of chemical graph theory.

Ivan Gutman