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BOOK REVIEW

Molecular Topology and Its Applications

by

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The book describes a large class of molecular–graph–based structure descriptors ("topological indices") and a large number of their chemical applications. Under "topology" (in the title of the book and elsewhere) is meant part of molecular structure that is represented by a molecular graph. The book is mainly concerned with matrices and matrix invariants associated with molecular graphs and, of course, their chemical applications.

The book consists of preface, nine chapters and eleven appendices. Each chapter is followed by a long list of references. Each part of the book is richly illustrated by figures, diagrams, and tables, so that the text is a pleasure to read and chemists will easily be able to follow and understand it.

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 should better consult a more extensive source.

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

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

The considerations in Chapter 3 are made more detailed 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 introduced variants. In other words, 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 of the authors (M. V. D.) did a lot of work in this area.

Also Chapter 6 is an "outlier". It presents the main notions and methods from statistics, needed for the construction of QSPR and QSAR models (which, in turn, provide the main chemical applications of the structure–descriptors considered in this book). The text of Chapter 6 is written in a concise, clear, and precise manner, so that – in the opinion of the reviewer – this part of the book may become a preferred starter to those who want to do 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 listed. It should be noted that the Szeged index is also a distance–based graph invariant, closely related to the Wiener index. In this chapter one author (P. V. K.) exposed almost everything what he did (and published) in connection with the Szeged index. The applications of the Szeged index in physical, medicinal, and environmental chemistry, pharmacology, and toxicology are remarkable. To give the reader of this review an idea we mention modeling polychlorinated biphenyls in the environment, characteristic vibration of carbonyl group, Mössbauer parameters, antituberculotic activity of quinolones, receptor binding potency of indolealkylamine, toxicity of nitrobenzenes, etc. etc.

Chapter 8 outlines the theory and applications of a close relative of the Szeged index – the so-called PI index.

Follows Chapter 9 entitled "*Exhaustive Information*", which embraces also the eleven Appendices. In this chapter a list of main chemical applications of the topological indices are given, with pertinent references, but without any further detail. 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 on prediction of physico–chemical property, biological activity, and toxicity, whereas Appendix 11 contains similar data on QSPR and QSAR models.

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 elements of chemical graph theory. For mathematicians the book may serve as a document of the applicability of various graph invariants, and as a source of such invariants worth their attention.

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