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Graph-Theoretical Matrices in Chemistry

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There are a few graphical representations of molecular structure (constitution) and hundreds of topological indices. However, to derive a topological index from a molecular graph, the first step is to construct its matrix, or to say it more explicitly, every molecular index rests on a graph-theoretical matrix. Thus, the third book in the series Mathematical Chemistry Monographs is devoted exclusively to matrices used in topological analysis of molecules.

The book generally deals with adjacency, incidence, and distance matrices. As every graph consists of vertices (V) and edges (E), there are, according to the second classification, two kinds of matrices, i.e., vertex- and edge-matrices. But these are very crude classifications; the book describes a total of 130 matrices, i.e., 17 kinds of adjacency matrices, 6 kinds of incidence matrices, 28 kinds of distance («and related») matrices, and 18 kinds of »special matrices» (Wiener matrices, reverse Wiener matrices, Szeged matrices, Cluj matrices, Hosoya matrix, path matrix, etc.). Chapter 6 of the book is devoted to graphical matrices, and shows how to derive topological indices from them.

Altogether, in its seven chapters (Introduction, The Adjacency Matrix and Related Matrices, Incidence Matrices, Distance Matrices and Related Matrices, Special Matrices, Graphical Matrices, and Concluding Remarks), 72 paragraphs, 205 pages, and 365 references, followed by the well designed Subject index, this small book gives to informed as well as to not-so-well informed readers a short, compact, and systematic overview over all kinds of matrices derived by chemical graph theory.

More than that is not to be expected. The book is conceived as a lexicon or manual, not as a textbook. Thus, the reader will not be instructed how to calculate topological indices from appropriate graph theoretical matrices. Further, it is not at first clear what these matrices are good for, and the reader will not find any systematic comparison of the various kinds of matrices. For instance, it is not clear how N-tuple, CAM and LDF codes are derived from graph-theoretical matrices, and it is not at all explained how to compute the connectivity identification (ID) number. For sure, the reader may find help in the referred literature, but in this respect the Graph-Theoretical Matrices in Chemistry cannot be regarded as a ready-to-use manual.

Some problems with this book stem from the fact that four authors participated in its writing, with their own styles and ways of presentation, which led to slight inconsistencies. For instance, the last paragraph on page 5 (Introduction) would be better placed in the Preface and the last paragraph in the Conclusion remarks. Also, poor coordination between the authors and the publisher resulted in a typing error on the front page (it is not clear whether the title of the book is Graph-Theoretical Matrices in Chemistry or Graph Theoretical Matrices in Chemistry). But, in spite of the errors and inconsistencies, I find this book a very successful and useful presentation of various kinds of matrices in use in molecular graph theory.

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