**MATCH** Communications in Mathematical and in Computer Chemistry

## **BOOK REVIEW**

## Introduction to Chemical Graph Theory

by

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Chapman & Hall / CRC Press, Boca Raton, 2019. Series: Discrete Mathematics and Its Applicatons, 259 pp. ISBN 9781138325081.

This book is mainly concerned with topological indices, a topic of great interest in chemical graph theory. As the authors indicate in the *Preface*, there is no intention of being comprehensive in the contents related to topological indices, but rather to make a careful selection of the most commonly used mathematical approaches. The book is written in a self-contained form, beginning with a chapter of *Preliminaries*, where they exhibit all the results on graph theory that will be used later in the book. Each chapter begins with a brief introduction on the origin of the topological index and ends with a list of exercises, ideal as a textbook for an introductory course on chemical graph theory.

The book is divided into five parts:

1 Preliminaries;

- 2 Distance in graphs and the Wiener index;
- 3 Vertex degrees and the Randić index;
- 4 Independent sets: Merrifield-Simmons index and Hosoya index;
- 5 Graph spectra and the graph energy.

In the *Preliminaries*, after a brief introduction on related graph theoretical terminologies, the authors give an overview of topological indices, together with the references where they first appeared. In *Chapter 2* topological indices based on distance are considered. Extremal value problems of the Wiener index and its variants over general graphs and over trees are studied. Several sections are mainly concerned with the the Wiener index in the class of trees with a given sequence of degrees or with a given sequence of segments. The chapter ends with a section on the inverse problem: given a positive integer n, can we find a structure (graph) with Wiener index n?

Degree-based topological indices is the topic in *Chapter 3*. The authors deal with these indices through a unified approach, by introducing a symmetric bivariate function f(x, y) defined over  $\mathbb{N} \times \mathbb{N}$ . Again they examine extremal problems for trees with a given degree sequence. In both chapters, *greedy trees* play an important role. Entire sections on the Zagreb indices and the ABC index are given in this chapter.

Chapter 4 is aimed at the Merrifield-Simmons index and the Hosoya index and its mathematical properties. The behavior of these indices when transformations are made to a graph are considered and then, applications to the extremal value problem in graphs and trees are given. The chapter ends with a study of the independent polynomial and the matching polynomial of a graph.

*Chapter 5* begins with an introduction to the spectral theory of graphs. The spectrum of the most important matrices associated to a graph are analyzed, such as the adjacency matrix, the Laplacian matrix and the signless Laplacian matrix. The rest of the chapter is devoted to the energy of a graph and its mathematical properties. Bounds and extremal problems for trees and graphs are considered for the graph energy and other energy-like invariants, such as matching energy, laplacian energy, the incidence energy, the Estrada index, among others.

The book ends with an extensive *Bibliography* containing 132 references and a short *Subject Index*.

In summary: The book *Introduction to Chemical Graph Theory* contains valuable information on topological indices, with emphasis on the extremal value problem on graphs and trees. It will undoubtedly be useful for beginners and experts in chemical graph theory.

Juan Rada