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BOOK REVIEW

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Mathematical Aspects of Randić-type Molecular Structure Descriptors

Mathematical Chemistry Monographs,
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One of the contemporary leaders in mathematical chemistry Professor Ivan Gutman (Faculty of Science, University of Kragujevac, Kragujevac, Serbia) produced, in collaboration with the Chinese mathematician Professor Xueliang Li (Center for Combinatorics, Nankai University, Tianjin, China), the first book in the series *Mathematical Chemistry Monographs*. In this book, the authors consider the original Randić connectivity descriptor that Professor Milan Randić proposed in 1975 and Randić-type descriptors. Immediately after being published, Randić's famous paper entitled "On Characterization of Molecular Branching" (*J. Am. Chem. Soc.* **97** (1975) 6609–6615) attracted attention of mathematical chemistry community, but also of computational chemists, environmental chemists, people doing research in drug design and many other chemists interested in encoding molecular structure by a single number, and later even by mathematicians such as Béla Bollobás and Paul Erdös. In due course, this paper became the most cited mathematical chemistry paper of modern times and was listed as the 95th paper in the compilation of 125 most cited papers that appeared in the *Journal of the American Chemical Society* in the last 125 years. While initially chemists used this index mostly in its original form, mathematicians later investigated its mathematical properties. The present book is about mathematical aspects of the Randić descriptor and its generalizations.

The book consists of six chapters and bibliography.

The first chapter, entitled *Introduction* (pp. 1–10), contains a foreword by Milan Randić, introductory notes, the outline of the book and basic terminology and notation.

The second chapter, entitled *The Randić index* (pp. 11–107) considers the Randić index in the original formulation:

$$R(\mathrm{G}) = \sum_{uv \in E(\mathrm{G})} [d(u)d(v)]^{-1/2}$$

where $R(\mathrm{G})$ is the Randić index of a graph G, u,v are vertices of G, $d(u)$ and $d(v)$ are degrees of vertices u and v, E denotes the number of edges in G and the summation goes over all pairs of adjacent vertices in G. Li and Gutman adopted the symbol R for the Randić index instead of the more commonly used χ. The chapter is divided into several sections, each dealing with a class of graphs. The considered graphs are general graphs, trees, unicyclic, bicyclic and tricyclic graphs, chemical graphs and chemical trees. Various mathematical properties, such as minimum and maximum values of the Randić index for some graphs, bounds for trees of a given order, bounds of some chemical graphs, *etc.*, are reported.

The third chapter, entitled *The General Randić Index* (pp. 109–273), considers the generalized form of the Randić index:

$$R_\alpha(\mathrm{G}) = \sum_{uv \in E(\mathrm{G})} [d(u)d(v)]^{\alpha}$$

where α is a real number. If we put the value $\alpha = -1/2$ in the above formula, then we get the original Randić index. On the other hand, if we put $\alpha = 1$, we get the second Zagreb index (see I. Gutman and N. Trinajstić, "Graph Theory and Molecular Orbitals. III. Total π-Electron Energy of Alternant Hydrocarbons," *Chem. Phys. Lett*. **17** (1972) 535–538; I. Gutman, B. Ruščić, N. Trinajstić and C. F. Wilcox, Jr., "Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes," *J. Chem. Phys.* **62** (1975) 3399–3405; for some reason these references are not cited in the book). Graphs considered are general graphs, unicyclic graphs, trees and chemical trees. And again, many mathematical properties, such as the trees with minimum and maximum values of the general Randić index, chemical trees with minimum and maximum values of the R_{-1} index, *etc.*, are discussed.

The fourth chapter, entitled *The Zeroth-order Randić Index* (pp. 275–309), reports on the properties of the Randić index of the zeroth-order:

$$^0R(\mathrm{G}) = \sum_{u(\mathrm{G})} [d(u)]^{-1/2}$$

and the general Randić index of the zeroth-order:

$$^0R_\alpha(\mathrm{G}) = \sum_{u(\mathrm{G})} [d(u)]^{\alpha}$$

where the summation in both above formulae goes over all vertices in G. The general zeroth-order Randić index for $\alpha = 2$ gives the first Zagreb index. In this chapter, the authors discuss general graphs with maximum ${}^0R$ and ${}^0R_\alpha$ indices of trees, unicyclic graphs with the first three extremal ${}^0R$ and ${}^0R_\alpha$ indices of chemical graphs and chemical trees.

The fifth chapter, entitled *Higher-order Randić Indices* (pp. 311–317), offers a short discussion about the *m*-th order Randić index:

$$ {}^mR(\mathrm{G}) = \sum_{i_1 i_2 \ldots i_{m+1}} [d_{i1} d_{i2} \ldots d_{im+1}]^{-1/2} $$

where the summation is over all paths $i_1 i_2 \ldots i_{m+1}$ of length *m*, contained in G. The ${}^mR$ is considered for general graphs.

In the last chapter, *Conclusion* (pp. 319–322), Li and Gutman state that they have examined various extremal problems related to the Randić index and its various generalizations. They were particularly interested in two problems: to find the lower and upper bounds for the Randić indices (R, R_α, ${}^0R$, ${}^0R_\alpha$, ${}^mR$, $m>1$) and to characterize graphs for which the Randić indices assume the extremal (minimum or maximum) values. In this chapter, the authors also pose a few open problems that they find most interesting and challenging from the mathematical point of view.

The book ends with *Bibliography* (pp. 323–330) containing 105 references given in alphabetical order. The Zagreb group papers, related to the subject of the book, are cited 5 times. It appears that the weakest point of this otherwise very carefully prepared book is the bibliography, because a number of relevant papers are not mentioned.

It is also announced that three more books in the series *Mathematical Chemistry Monographs* are already in press. Information about these three forthcoming books can be found at the address http://www.pmf.kg.ac.yu/match/. We are looking forward to other books in the series with great anticipation because the first beautifully designed book is so rich in interesting and stimulating results.

Nenad Trinajstić