International Journal of Quantitative Structure-Property Relationships
Volume 2 • Issue 1 • January-June 2017

Book Review

Solved and Unsolved Problems of Structural Chemistry

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Solved and Unsolved Problems of Structural Chemistry
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472 pp.
$104.00
ISBN 978-1-4987-1151-7

This book covers the basic aspects of mathematical chemistry involving chemical graph theory, with special emphasis and reference to the work of Prof. Milan Randić. It presents the history and evolution of chemical graph theory and its contribution to structural chemistry, problems faced by the researchers in chemical graph theory in general, and personal experiences of Prof. Randić in his research career on Chemical Graph Theory. This book illustrates Prof. Randić's ideas, contributions, philosophy, arguments and also the disputes related to his work. This book is not just a description of scientific terms, formulae and algorithms, but also a mirror of scientific contributions and research of Prof. Randić. It is a thoughtful collection of scattered information outlining different tools and techniques from discrete mathematics that can be used to address comparatively less understood problems in chemistry.

The Foreword of the book has been written by another legendary scientist Prof. Alexandru T. Balaban, while the Preface has been contributed by the three authors of the book. Chapter 1 gives an introduction to the role of Mathematics in structure-property relationship problems. The readers are given the concept of mathematical chemistry with several examples and discussions on solved and unsolved problems in chemistry. Chapter 2 goes deeper with more technical details of mathematical chemistry and introduces the Graph Theory. Chapter 3 presents a more detailed discussion on Graph Theory in the context of Kekule valence structure and Hückel Molecular Orbital Theory. The molecular structure representation using Graph Theory is elaborated with several examples. Chapter 4 outlines the construction and several properties of the characteristic polynomial, one of the basic attributes of graphs used in Graph Theoretical approaches. The topic is covered with several examples, illustrations and exercises. Chapter 5 deals with chemical structure representation, quantitative structure-activity relationships (QSAR), regression analysis and some problems of QSAR. Although this chapter is not very comprehensive, it gives a preliminary concept of QSAR to the intriguing

minds of active researchers who are new to the field. Chapter 6 discusses on molecular descriptors, more specifically, the different types of connectivity indices which originally evolved from the work of Randić and/or related to the approach of Randić. Chapter 7 introduces the concept of partial ordering, an important concept of discrete mathematics, which according to the authors has been mostly overlooked in the QSAR community except for scientists in chemometrics, chemical graph theory, and mathematical chemistry. Chapter 8 depicts some comparatively newer versions of different metrics and corresponding molecular descriptors. The next chapter focuses on analysis of similarity of molecules and search of combinatorial libraries using molecular descriptors. Chapter 10 discusses on theoretical aspects of aromaticity with special reference to polynuclear systems. Chapter 11 focuses on Clar's approach of the aromatic sextet theory. Chapter 12 considers calculation of ring currents in polycyclic conjugated hydrocarbons based on the conjugated circuit model. Chapter 13 discusses on application of Graph Theory in Bioinformatics. Chapter 14 gives examples of a few unrecognized works of some significance and importance that remain overlooked and unrecognized for some time by most scientists even though such works may have received limited citations. At the end, there are 23 appendices, some of which describe the Prof. Randić's own experiences of responses received from different Journal editors and/or reviewers on his structural chemistry research.

This book is a unique piece of work showcasing the work, philosophy, contributions and experiences of Prof. Milan Randić in the context of his research in the field of Mathematical Chemistry. It discusses many comparatively less understood and less discussed problems in Chemistry connected to topics such as the notion of aromaticity and conjugated circuits, the generalized Hückel $4n + 2$ Rule, etc. and relate them to Randić's own work. The beauty of the book is that it discusses the problems in the form of several examples avoiding the details of mathematical treatments in order to make the topic clear to the novice readers. The discussions and arguments presented in the book will kindle the interest of new researchers to go deeper into the topics of the solved and unsolved problems of chemistry. Both newcomers as well advanced researchers in the field of Mathematical Chemistry will be benefitted from the lucid and explanatory presentations of the topics. The coverage of the book, however, mainly concentrates around the contributions of Prof. Milan Randić and related work. A reader, thus, should not expect to have a comprehensive coverage of all topological descriptors and related work in this book. Nevertheless, this book presents a detailed information on the work contributed by Prof. Randić and the basic concepts of Mathematical Chemistry in an unparallel fashion making it a very useful resource for the researchers in the field.

Kunal Roy is a Professor in the Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India. He has been a recipient of Commonwealth Academic Staff Fellowship (University of Manchester, 2007) and Marie Curie International Fellowship (University of Manchester, 2013). The field of his research interest is QSAR and Molecular Modeling. Dr. Roy has published more than 250 research papers in refereed journals. He has also coauthored QSAR related books entitled "Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment" (Elsevier, 2015) and "A Primer on QSAR/QSPR Modeling: Fundamental Concepts" (Springer, 2015) and edited "Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment" (IGI Global, 2015). His current h-index is 34.