BOOK REVIEW

Solved and Unsolved Problems of Structural Chemistry

by

Milan Randić, Marjana Novič & Dejan Plavšić

In spite of its title, this book is on mathematical chemistry, mainly (but not exclusively) on chemical graph theory. This is an unusual and unconventional piece of work. To borrow an expression from the book itself, it is *illustrious*, in the sense of *being notably or brilliantly outstanding because of its achievements*. We explain and exemplify this in the later parts of this review.

First a formal description of the contents:

The book begins with a *Foreword* written by Alexandru T. Balaban, a *Preface* written by the three authors, and the authors' short biographies. The main part of the book is divided into 14 chapters:

1. *Introduction* (pp. 1–21)

2. *Mathematical Chemistry* (pp. 23–65)

3. *Graph Theory and Chemistry* (pp. 67–100)

4. *Characteristic Polynomial* (pp. 101–130)

5. *Structure–Activity* (pp. 131–149)

6. *Molecular Descriptors* (pp. 151–197)

7. *Partial Ordering* (pp. 199–218)

8. *Novel Molecular Matrices* (pp. 219–245)

Each chapter ends with a long and exhaustive list of references.

At the end of the book, there is a *Subject Index* (pp. 461– 467) and a *Name Index* (pp. 469–472).

However, remarkably, after the Chapter 14 we find 23 (twenty three!) *Appendices* (pp. 397–459), offering such outlandish information as the "*Detection of the Illegal Deck of Cards for Graph Reconstruction*", "*First Page of the Book of Euclide*", "*Full Quote of Immanuel Kant*", "*Eigenvalues and Eigenvectors of Hexatriene*", "*Halogen Compounds and Their Boiling Points*", a quotation from "*Nature*" from 1974, and an "*Input and Output of the Program VESPA*". On the other hand, most of these appendices are related to the authors' (or more precisely: to Randić's) disputes and arguing with those who were "*hostile*" towards chemical graph theory. More on this matter later.

Chapters 4–13, and to some extent also Chapters 2, 3, and 14, present the ideas and scientific contributions (or, if I may say: the opus) of Milan Randić, the results of his long and extraordinarily productive scholarly activities. Each of these chapters corresponds to one of Randić's research interests. His own results are outlined in full detail. Other, sometimes closely related, researches and other colleagues' contributions are covered much less extensively. A characteristic example is Chapter 6. In spite of its title "*Molecular Descriptors*", of the several dozens of important such descriptors and several hundreds of existing such descriptors, only one is considered. As one may expect, this is the connectivity index, which most scholars nowadays call *the Randić index*.

Chemical graph theory is a scientific discipline that has and should have a mathematical content. The book "*Solved and Unsolved Problems of Structural Chemistry*" is written in such a manner that the mathematical formalism is reduced to a minimum, and is mainly made clear by means of examples. By this, the book will be welcome by those (numerous) readers who do not master and do not like abstract

mathematical formulas and boring proof techniques, and who prefer examples and pictures. In other words: this book is written for a readership of chemists (together with biologists and pharmacologists). Mathematically oriented readers may, on the other hand, be motivated to formalize the results and claims found in the book. Of course, many of the missing mathematical treatments exist in the references quoted.

Already in the *Preface* (on page XIII) the authors declare that their book is "*unusual and unconventional*". Indeed it is! Contrary to many other existing monographs concerned with chemical graph theory or its selected special topics, this book is full of interesting, unusual, and surprising excursions, making its reading a great pleasure. Everywhere in the book, we find historical details and anecdotes, related to physics, chemistry, physical chemistry, and mathematics, often coming from Milan Randić's personal experience. Colleagues interested in philosophy of science (or philosophy in general) will also find a wealth of intriguing ideas. For these colleagues we especially recommend Chapter 14, and its sections "*On Beauty in Science*" and "*Sleeping Giants*". The same chapter will be a gold mine for scholars interested in the history of chemistry.

At the very beginning of the book (on pp. 3-5), we encounter such seemingly unrelated topics as the three Greek mathematical problems of antiquity (doubling a cube, trisecting an angle, squaring a circle), followed by the history and presentation of the four-color-problem in graph theory (pp. 5-6). A few pages later are outlined the famous Hilbert Problems in mathematics. On page 365 is a short story of Georg Mendel's discovery in genetics. What some appendices contain has already been mentioned. As the last example of this kind, we return to Chapter 6: In its middle there is a short essay on the great Croatian scientist Ruđer Bošković (1711–1787), whose relevance for molecular descriptors is not easy to envisage.

Another thing that makes the book "*Solved and Unsolved Problems of Structural Chemistry*" unusual and unconventional are the countless cases when the author (i.e., M. R.) argues with his existing or imagined opponents and "enemies" of chemical graph theory. The most explicit parts of the book are the Appendices "*Early Hostility toward Chemical Graph Theory*", "*Editorial Alert to Reviewers on Graph Theoretical Manuscripts*", "*Hostile Report of Anonymous Referees on Novelty in Graphical Bioinformatics*", "*Late Hostility toward Chemical Graph Theory*", as well as Appendix 3 concerned with an negative report on one of M. R.'s papers, by an incompetent ref-

eree. An interesting idea in the book is that among scientists there are "tool makers" and "tool users". With regard to this, the authors say: "*Toolmaking, which has been one of our longtime interests and a longtime misunderstood activity, is unfortunately not well appreciated among tool users.*"

Everybody who did research and tried to publish papers in chemical graph theory, experienced difficulties and hostile reports by referees hidden by the veil of anonymity. This certainly applies to the author of the present book review. However, most of us would "swallow" the problem, and silently try again at some other journal or publisher. Not Milan Randić! His fights with the reviewers and editors are legendary. Relevant details of these controversies are now reproduced in the book. We also learn that analogous difficulties were (and still are) encountered by scientists working in other new, not yet established and officially recognized, fields of science.

In this reviewer's opinion, the true judge of the scientific relevance and practical applicability of the results of chemical graph theory is *Time*. If what we are doing and producing has a true scientific value, then this will be – sooner or later – recognized, no matter of what the opinion of the hostile contemporary majority is. If, however, what we are doing and producing has no true scientific value, then this too will be – sooner or later – recognized, irrespective of the eloquence are zeal of its defenders. The sad fact is that *Time* needs time, whereas our personal time is limited.

No doubt that the authors of the present book would disagree with such an opinion.

Back to the book:

In summary, "*Solved and Unsolved Problems of Structural Chemistry*" is a valuable treatise, outlining practically all facets of the research of Milan Randić in various areas of chemical graph theory. In some sense, this is a memory which Milan Randić has erected for himself (helped by his two coauthors). Considered as the newest monograph on chemical graph theory, this book is worth purchasing and should be recommended for any decent science library. However, in view of its unique approach not only to chemical graph theory, but to scientific research and science in general, and bearing in mind the wealth of bizarre and apparently unrelated scientific details, this book should be a valuable item in the personal library of all those who ever did any work or ever had any interest in chemical graph theory.

Ivan Gutman