Review: eBook Bentham Books

Eds: S.Basak, G. Restrepo, J.L. Villaveces….

Title: Advances in Mathematical Chemistry and Applications, Volume 1.

All chapters of the book provide lists of abbreviations, extensive lists of references as well as indexes for a quick access to the various concepts of mathematical chemistry.

What is Mathematical Chemistry? A personal view: 50 years ago I asked a professor in organic chemistry to be allowed to study more mathematics; at that time his answer was: “What should mathematics in chemistry be good for?” However, about 300 years ago, Kant (1724-1804) argued that mathematics must be an essential part of any chemical activity, if chemistry is to be called a science. Kant changed his mind regarding chemistry when the first mathematical concept, i.e., that of mass-balances by Lavoisier became a basic principle in chemistry.

Looking today in the scientific chemical literature almost everywhere a relation to mathematical aspects can be observed. Hence, there is much mathematics in chemistry but does this represent mathematical chemistry? Can theoretical chemistry or chemical physics (the more mathematical oriented way of viewing on physical chemistry) be denoted mathematical chemistry? Definitely to some degree; however, both are parts of mathematical chemistry but not mathematical chemistry itself. Is chemoinformatics or chemometrics mathematical chemistry? Again, to a certain degree yes; especially chemoinformatics with its focus on algebraic relations seems to overlap strongly with the area mathematical chemistry. An answer can be found in a recent book edited by S. Basak, G. Restrepo, and J.L. Villaveces. The book intends to awake an interest for a broad group of potential readers that comprises not only mathematicians or mathematical interested scientists. They write in their preface: “The branches of mathematics considered are graph-, information- and categories theories, as well as statistics, fuzzy sets, network analysis, classification techniques, ordering, topology, neural networks and mathematical aspects of molecular dynamics and quantum chemistry.” The key words appear to be “mathematical aspects of…”. Thus to define mathematical chemistry it is suggested to be *'the science of structural mathematical aspects inherent in chemistry'*. In that sense chemistry could be restructured by the main mathematical methods which are applied. Analytical chemistry may serve as an example as it has mathematical aspects that have to do with algebraic field theory and its application to highly nonlinear algebraic equations. Another example could be chemical thermodynamics with broader application of Pfaff forms (theory of differential forms), etc. Any chemical class (the definition and discussion of chemical classes and their applications is one of the main tasks in chemistry) can consequently be seen as equivalence classes and the crucial point is obviously the selection of the best equivalence relation and furthermore the way as to how far equivalence classes can be related to each other (which could be a task of the mathematics of order relations, by crisp or fuzzy-techniques).

With this in mind rather high expectations prevail when the reader starts to dive into this new book about “Advances in Mathematical Chemistry and Applications”. Briefly said, I am impressed of the contributions to the book and in several cases it was a pleasure to study specific chapters. Clearly certain locations in the texts were disclosed, where I would suggest some extensions or (more seldom) an abridgement and clearly typos were found although I did not look specifically for this kind of bugs. Anyway, it would be too pedantic to list my few points of improvements or criticisms in front

of this indeed well-done book. However, before publishing a possible second edition a carefully reading and updating should be done.

A main part of the book informs about an algebraic relation, a binary relation, which is the basis of a graph theoretical representation of molecules. Graphs can be drawn in different ways; consequently, the mathematical basis for chemistry is the search for graph invariants. Graph invariants, also known as topological indicators or descriptors, are discussed in several chapters, some with respect to applications like the very important field of Quantitative Structure Activity/Property Relationships (commonly abbreviated as QSAR or QSPR), or with the focus on the necessity of generating new topological indicators. Also chapters are suitable for students simply due to the fact that the use of topological indicators is well explained. They really could serve as motivation for students.

Classification is also a matter of the level of similarity that one is accepting. In modern drug design similarity based search programs play a crucial role. This book provides a chapter, where recent advances in this context are discussed. Thus, both “similarity-based virtual screening” as well as Bayesian networks is discussed and an interesting view on the well-known Tanimoto-coefficient can be found.

When classification is demanded, binary relations are again of importance. Two chapters are devoted to ordering. In one chapter the study of directed acyclic transitively reduced graphs is in focus; however, not only the mathematical structure of partial orders, but also the algebraically more comfortable structure of lattice theory is applied. It is shown that partial order can be helpful in prediction of properties of chemical substances and especially lattice theory allows another approach than by graph-theoretical invariants to relate structural information to chemicals properties, e.g., mutagenicity. An additional chapter that could be seen as a logical consequence of partial ordering argues that any partial order implies a comparability graph, which is a realization of the relational character inherent in chemistry. This chapter bridges the gap to the chapters about topological indicators by analyzing the similarity among comparability graphs (for instance by the graph edit distance). Therein the comparability graphs are results of order relations between topological indicators.

Classification and ordering render bridges to two other concepts, discussed in this book. The simple question, how many isomers of a given compound exist was already asked in the 19^{th} century opening a new field of applications in chemistry, i.e., group theory or still more correctly theory of finite group actions. More general the question focus on the basic chemical concept of classes has its counterpart representing deep chemical thinking, i.e., what kind of stoichiometric information determines uniquely a set of chemicals, when a set of valences is defined by the users of the program, described in this chapter (MOLGEN). A further concept which has had an unequivocal impact on chemistry is the concept of periodicity. Also here it is possible to relate classes of chemical entities to each other. The reader is thus transferred to the world not only of classical chemical concepts, but also to the fascinating world of elementary particles. The particles are classified (getting a name) and their relations to other particles (the periodicity) are identified, often through construction principles, which resemble early concepts such as the platonic polyhedras.

Chemistry is the science of reactions. To understand reactions classification, similarity measures and topological indices may be used. However, the very nature of the aforementioned concepts is static. A chapter at the heart of chemical reactions, either thermodynamically considered or in terms of reaction kinetics explains the recent advances in application of the density functional theory (DFT).

Many fruitless debates about electronegativity, softness/hardness and other heuristic concepts could apparently be replaced by concepts derived from DFT.

To summarize, the book offers in a well-balanced manner, modern aspects of mathematical chemistry. Nevertheless, some few points appear striking, which are not directly related to the 26 single chapters, but have to do with the conception:

1) the nice idea of relating the chapters / authors by directed graphs at the very beginning of the book is fine. However,

a) the reader would wish more internal relations. I know, it is extremely hard for editors to do this because this would be an n+1th iteration of the editor's work. Nevertheless, by a network of mutual referencing within the book chapters the book could be by far more than the sum of its chapters.

b) it is striking that these graphs contain concepts, which are at least in this volume not mentioned as for example category theory

2) The title “Advances in Mathematical Chemistry…” makes clear that -clearly- not all aspects of mathematical chemistry will be found in this book. Nevertheless, I had expected to find aspects mentioned which (in my eyes) belong to mathematical chemistry such as

- Chirality, mixing character and branching concepts, which are discussed in seminal papers of Ruch, where majorization and the concepts of Young diagrams play a role.
- Semiempirical concepts, based on easy accessible information, which are helpful for forecasting chemical reactions.
- Chemical networks, their evolution and their invariants

3) Many mathematical concepts are only realizable, when powerful computer power and appropriate software are at hand. In this book many important software-packages are mentioned. An appendix with a list of software, their main aim, their availability and some main computational requirements could improve the book.

As a conclusion, I can recommend this book not only for students, but also for chemists and mathematicians. Maybe my old professor of organic chemistry should read this and hopefully forthcoming volumes, too. It might persuade him to change his mind about mathematics in chemical science!

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