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Theoretica Chimica Acta

Book reviews

Klein DJ and Randic M (eds) (1990) (Proceedings of the 3rd International Conference on Mathematical Chemistry, Galveston, TX (USA), March 1989) Weinheim, VCH Publ, Weinheim, FRG

This book is identical with a special issue of the Journal of Mathematical Chemistry. Such special issues are usually not a subject of book reviews and there are strong arguments against reviewing conference proceedings. Scientific papers should be published in ordinary journals where consistent refereeing is guaranteed and the para-literature of conference reports and technical notes should not be upvalued. Not to mention the problem for an editor to find a competent reviewer if all experts in the field are authors of the book.

Why then a review in this special case and why review, so to say, the Journal of Mathematical Chemistry in Theoretica Chimica Acta? This is an occasion to clarify the relation between Mathematical Chemistry and Theoretical Chemistry. They are definitely not independent or distinct domains, but Mathematical Chemistry is a branch of Theoretical Chemistry. This is sometimes obscured by the tendency to identify Theoretical Chemistry with Quantum Chemistry, another, though admittedly important, branch.

How do the representatives of Mathematical Chemistry see their field? In spite of a remark in the editorial, that the conferences to which this one belongs gradually change their character, there is still an overwhelming dominance of the application of graph theory to chemical problems. The few papers (e.g. by Paldus or Matsen) on the N-electron problem don't really fit into the general pattern. There are, of course, various applications of graph theory, but the classical field of the graph theoretical reformulation of the Hückel MO theory of conjugated polycyclic hydrocarbons plays a central role together with the general problem of enumeration of structures.

The reviewer, a theoretical chemist with some affinity to mathematics, who does not feel competent to report on all papers in detail, wonders where the train of mathematical chemistry is going, and to which extent it will in the future contribute to a theory of chemistry. Will Mathematical Chemistry remain centered around Hückel theory and molecular topology?

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Liebman J. F. and Greenberg A. (eds) (1989) From Atoms to Polymers. Isoelectronic analogies. VCH Publ., Weinheim, 473 pages, DM 218.

This is one of the volumes of the series 'Molecular structure and energetics' edited by the same authors. More than ten volumes have already appeared, each consisting of independent chapters by different authors. Of the ten chapters of this book five are basically theoretical, one by R. F. Bader, R. J. GIllespie and D. J. Mac-Dougall on the VSEPR model in the light of the concept of the Laplacean of the Charge Density, one by G. Frenking, W. Koch and J. F. Liebman on He-containing molecules, one by D. M. Schrader and R. C. Wedlich on the binding of positrons and muons to atoms and molecules, one by C. K. Jørgensen on the chemistry of systems containing unsaturated quarks and one by S. A. Kafafi and J. P. Lowe on substitutional effects on polymer band gaps. The

chapter by Bader et al. is likely to be read with great interest by those who have been puzzled by the many rationalizations or predictions of chemical structures by a model that at first glance has little to do with quantum mechanics. The chapter of Frenking et al. hopefully serves to demystify the helium chemistry. Quantum chemical computer programs have no difficulty with molecules in which H is a replaced by the isoelectronic He^+ ion. Schrader's and Wedlich's chapter appears to give a rather complete bibliography (276 references) on positronic and muonic molecules. Jørgensen speculates about the possible existence of fractionally charged atoms. Kafafi and Lowe argue mainly in terms of a qualitative MO theory.

Even the six other experimental chapters are a source of challenging information for a theoretist. N. Burford, J. P. Passmore and J. C. P. Saunders report on homopolyatomic cations of groups 16 and 17, like S_8^{2+}, O_2^+ or Cl_3^+. D. D. M. Wayner and D. Griller describe electrochemical studies of transient (mainly organic) free radicals e.g. alkyl or alkoxy. J. K. G. Watson contributes a chapter on hydrides like H_3, NH_4 that are bound in excited states. The technologically interesting topic of molecular electronic devices is treated by F. L. Carter and R. E. Siatkowski. The last chapter by M. W. M. Hisham and S. W. Benson is devoted to the estimation of the enthalpies of formation of solid salts.

The layout is pleasant and the hardcover completes the seriosity of the presentation.

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