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Recensiones

John Avery: The Quantum Theory of Atoms Molecules and Photons. London: McGraw Hill, 1972, XV + 378 pp., £ 5.50, or 8.00, respectively.

This book which, according to the author's own statement, attempts to be mathematically self-contained, leads the reader, in mere 370 pages, all the way from the explanation of the differential quotient to quantum mechanics of atoms and molecules, and further on the steep path up to the interaction between matter and quantized radiation fields. Basic mathematical knowledge (including an elementary introduction) plus classical mechanics are offered in 90 pages; general quantum mechanics, in 80 pages; atoms, molecules and crystals (including vibration and rotation) occupy a space of 130 pages, and the theory of radiation, 70 pages.

It goes without saying that this voluminous program cannot be treated rigorously and methodically on such a limited space. The author was compelled to procede as in a lecture held for beginners – colourful and emphasizing the basic ideas (by the way, enriching his text with historical details). The sequence of the first few chapters shows this clearly enough: gravitational law – differential and integral calculus – equation of motion – Leibnitz and Bernoulli.

The author certainly has devoted himself to his task with much engagement and enthusiasm. It seems that the book is partly the outcome of a series of lectures held for undergraduates. I do not know whether it will be met with too much interest. People who are especially interested in the theory of molecules will normally have a better command of mathematics and therefore tend to use more elevated books, the more so as the central part of Avery's text is rather short. Postgraduates interested in simple applications of the theory would, on the one hand, have to read a relatively long introductory part, in which the fundaments laid in lectures of mathematics and physics during the first few semesters are not exhausted fully, and the third part of the book would be to far-reaching to him. For those interested in gaining "general education" in theoretical chemistry, the situation is similar. For this reason, one must be afraid that the book will not fit cleanly into the course of ordinary university studies.

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P. O. Löwdin: Advances in Quantum Chemistry 6. p. XVI + 413, New York-London: Academic Press 1972, 29.50 $.

This series is now well established. It has proved over the years as a most valuable asset to quantum chemists for reference purposes. This can be credited to the editors intention to cover a very broad range of interests in the field of quantum chemistry. This time the articles contain the following subjects.

The introductory chapter is by John C. Slater and deals with one of his favorite subjects, the $X\alpha$ self-consistent field method. The article gives an objective historic review on the early work by himself and Gaspar. The author then tries to clear up misconceptions concerning the method, before he proceeds to discuss the specific advantages. He stresses the importance of this approach by a collection of 44 pages of references with applications, compared to 42 pages of the article itself.

The following chapter is also on a method which goes back a long time: the loge theory by Daudel. C. Aslangul, R. Constanciel, R. Daudel and P. Kottis discuss the implications of localizability of electrons in atoms and molecules. The concept of regions in space attributed to electrons or electron pairs is undoubtedly appealing to the chemist. Difficulties in the definition of regions as well as in practical use seem to have been partially removed. A new look at covalent and dative bonds appears to grow out of this concept as a noteworthy result.

D. J. Caldwell and H. Eyring investigate the potential of the Faraday effect for vibronic spectra and the structure of molecular excited states in an article on magnetic circular dichroism and diamagnetic molecules. They argue that the insensitivity of the Faraday effect to small changes in the wavefunctions provides a tool to determine the predominant features of wavefunctions. S. Basu and P. Sen discuss the Tomonaga theory of collective motion of quantum mechanical systems for the case of π-electron systems. Following the free electron gas model they feel that the aromatic hydrocarbons provide a system of two-dimensional collective oscillations. In particular, single-electron transitions are discussed on the basis of two-dimensional dipolar oscillations. H. Fujimoto and K. Fukui are concerned with the MO theory of chemical reactions. The frontier orbital approach serves again as a basis for a qualitative discussion, this time for charge-transfer interaction with regard to molecular deformation, orientation and bond interchange. A unified treatment of van der Waals forces between two molecules is the topic of B. Linder's and D. A. Rabenold's article. Their treatment is based on the reaction-field technique developed by Linder and it is suited for large molecular systems. Time-dependent perturbation theory, generalized susceptibilities and Kubo formalism enter as basic elements.

The last few articles deal with the more traditionally emphasized aspects of present quantum chemistry. Natural orbitals are presented by E. R. Davidson for two-electron and "few" electron systems. It appears that the advantage of rapid convergence is offset by the problem of finding good natural orbital approximations. Density matrix formalism is reviewed by K. Ruedenberg and R. D. Poshusta. Emphasis is placed on the orthogonal function approach following the work by Yamanouchi and Kotani. F. Weinhold's article deals with the important topic of upper and lower bounds to quantum mechanical properties. A general procedure is described to obtain these bounds from determinantal inequalities. The properties discussed include energy, scattering phase shifts, overlap, transition moments and second-order properties. *Ab-initio* calculations on large molecules are the subject of R. E. Christoffersen's paper. It might serve to bridge the gap to experimentalists, particularly organic chemists' interest. A survey of molecular systems shows the present day limits. The author expresses hope that the molecular fragment approach will enable us to go beyond.

The articles of this volume do not only cover a broad range of subjects but also vary considerably in length. This, however, does not necessarily mean popularity or importance of a topic rather reflects the editor's generous attitude with regard space limitations.

Karl Jug

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