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Book Review

A. C. Hurley: Introduction to the Electron Theory of Small Molecules. London, New York, San Francisco: Academic Press 1976, 340 pp., price: US $26.25 (£12.00)

This book is the first volume of a series of two presenting a systematic and consistent treatment of the electronic structure of small molecules. This volume serves as an introduction to the second part entitled "Electron correlation in small molecules", it covers the range from the formulation of the variation principle up to Hartree–Fock–Roothaan theory of small molecules.

After three introductory chapters on potential energy curves and surfaces, the variation principle, and symmetry properties of electronic wavefunctions, the first part of the book is devoted to a very thorough discussion of the structure of H_2^+ and H_2. Nearly all of the relevant methods ever tried to describe the two systems are presented and analyzed, starting from the simplest LCAO description of H_2^+ up to the natural orbital expansion for H_2. In this context, a detailed discussion of the importance of electron correlation for the behaviour of the H_2 potential curve is included – though correlation effects are generally not the subject of this volume.

The second half of the present book contains a discussion of determinantal wavefunctions and the development of the Hartree–Fock theory for closed- and open-shell atoms and molecules. The merits and shortcomings of this approximation for various properties such as total energies, binding energies, ionization potentials, dipole moments etc. are analyzed in detail and illustrated by many numerical examples, mainly on atoms and diatomic molecules.

The author leads the reader who is familiar with conventional Schrödinger quantum mechanics and the elementary theory of atoms an easily viable way into molecular quantum mechanics. The principles and methods used to describe the structure of small molecules are developed in a consistent and systematic fashion. Particular emphasis is laid on those methods which are used in numerical applications.

It must be noted that this book is not a textbook on valence theory. Aspects of chemical bonding in molecules are not taken care of at all. Though this is advantageous in order to keep the text as concise as possible, it is a little strange that Ruedenberg's pioneering work on the mechanism of the chemical bond in H_2^+ is not mentioned in the long chapter on H_2^+. On the other hand, one can find some material closely related to the main subject, but generally not treated in textbooks on quantum chemistry: Rydberg–Klein–Rees curves; Hellman–Feynman formulae and theorems; the symmetry paradox in approximate molecular calculations and so on.

There is one severe objection against Hurley's book: it is slightly old-fashioned and could have been written ten years ago. This concerns the selection of the methods presented, but much more so the numerical examples: despite of the rapid progress in numerical quantum chemistry during the last years, the book (appearing 1976) contains barely a single reference to a paper published after 1971. This is also an indication for the fact that the basic principles and ideas in quantum chemistry are still the same as they were twenty years ago and that the great progress in numerical applications did not add very much to our understanding of chemistry.

In conclusion, one can recommend Hurley's book to everybody who is interested in doing or understanding quantum chemical calculations on small molecules.

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