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Book Reviews

John P. Lowe: Quantum Chemistry. New York–San Francisco–London: Academic Press 1978. 600 pp., price: $49.50/£32.15

In the preface, the author states that this book is intended for use as a text accompanying an introductory one- or two-semester course on quantum chemistry. Accordingly, almost one third of the book consists of preparatory chapters on the physical foundations including quantum mechanics itself. The author solves this problem by a strong limitation of the material treated; of the quantum chemical methods, only the MO theory of the ground state of molecules is discussed, and the book is necessarily rather selective as far as applications of theory are concerned.

The author tried, with good success, to describe extensively those details which, according to experience, are difficult for the student. The pedagogical structure of the book also becomes evident from the large number of exercises, the solutions to which are partly given in an appendix. The overlap with similar textbooks, the number of which has been steadily increasing lately, is quite naturally large; nevertheless the book can be recommended on account of quite a number of well-presented details (such as e.g. the Walsh diagrams with their very nice orbital pictures).

W. A. Bingel, Göttingen

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S. Fraga. K. M. S. Saxena and M. Torres: Biomolecular Information Theory. Amsterdam: Elsevier Scientific Publishing Company 1978, X + 272 pages, price: US-$48.75

The scope and contents of this book are summarized in the authors' preface where they say: "Biological processes imply a mutual recognition of the systems involved, whereby the information stored in a system (or systems) is read by the other(s)... Quantum-mechanical research has yielded, over the years, an astonishing wealth of data on biomolecules or their submolecular components and the time has now come for a detailed inspection of the problems associated with recognition processes". The book is divided into four main chapters. Chapter one is devoted to the code and its origin and deals with molecular evolution, including mathematical models for the prebiotic formation of biopolymers. Chapter 2 deals with the molecular information theory, including the study of recognition processes in terms of stabilization energy, interaction sites, solvation effects. The next chapter treats in more detail the computational method for evaluating interaction energies, extending to clusters and Monte-Carlo techniques. The last chapter presents results of computational simulations including a detailed reproduction of results of conformational computations, essentially those of the reviewer, on amino acid residues of proteins and components of nucleic acids. It includes a description of minimization technique with an attempt of application to cyclic depsipeptide ionosphores.

The reader will find in this book interesting and stimulating information. He will also realize how far still is the problem from being solved.

B. Pullman, Paris

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M. F. O'Dwyer, J. E. Kent and R. D. Brown: Valency. New York–Heidelberg–Berlin: Springer-Verlag 1978, XI + 259 pp., price: US-$11.75

This booklet has been written to introduce undergraduate students into the field of chemical bonding. The authors try to develop approximate, pictorial approaches for the understanding of binding energies and geometries without using mathematics. After having introduced the SI units and also those ones more common in molecular physics, Chapters 2 to 4 (79 pp.) are devoted to the theory of atomic structure. The wave-picture is introduced, atomic orbitals and energy levels are extensively discussed and used to explain the ground configurations of atoms, the periodic system and the trends in different atomic properties. The central part of the book (Chapter 5, 83 pp.) treats the various aspects of chemical bonding on a qualitative level. The following topics are touched: MO and VB schemes, crystal field model, ionic binding, hydrogen bond, van der Waals forces, valence electron pair repulsion. Real and complex, localized and delocalized forms of orbitals are mentioned. The final two chapters (63 pp.) deal with bonding and structure of solids, and with spectroscopic methods (absorption spectroscopy from the radiofrequency to the UV range; mass spectrometry; X-ray-, *e*- and *n*-diffraction; photoelectron spectroscopy, however, is not mentioned).

Layout and presentation are appealing. The theoretical ideas and models are illustrated by tabulated empirical data. Every chapter is terminated by a summary and a set of problems.

The aim mentioned in the preface, namely "to avoid making erroneous statements in the interest of simplicity" might have been easily reached if the authors would have bestowed more care on their manuscript. The referee was especially disappointed at the figures. Most orbital plots in Chapter 3 are erroneous; the 2*p*-AO's seem to have infinite slope at the origin, $r^2\varphi_{1s}^2 \sim r^2\varphi_{2p}^2 \sim r$ for small r, the orbital lobes of *p* and *d*-AO's show incorrect shapes and magnitudes. Several force arrows in Fig. 5.7 have the wrong direction, the splitting of the Ag beam in the Stern–Gerlach experiment (Fig. 4.6) is strongly asymmetric, etc. The text contains some unusual formulations, too. E.g. the electron spin is "due to nonspherical distribution of charge and mass within its small size". When explaining the origin of the covalent bond, kinetic energy is not discussed at all. The normalization factor is suppressed in the LCAO-ansatz for the MOs. Ligand field splittings as well as the hydrogen bond are reduced to electrostatic effects without even mentioning overlap effects. On page 113 the authors quote experimental evidence on N_2^{2-}. "Because of the huge variation in energy, the ordinate" in the plot of atomic orbital energies versus Z "is $(-E)^{1/2}$ *and* logarithmic" instead of simply logarithmic. One of the given formulae (Paulings relation of bond energy and electronegativity) is wrong. The names of Kirchhoff, Ångström and Schrödinger are misspelled.

Only after revision I would recommend this book among others in the introductory course on the chemical bond.

W. H. E. Schwarz, Siegen

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D. B. Cook: Structures and Approximations for Electrons in Molecules. Chichester: John Wiley & Sons Limited 1978, 295 pp., price: £13.50

After having introduced the Hartree-Fock and Roothaan equations the author gives pictorial interpretations of molecular integrals, occupation numbers and orbital energies. Then he deals with AO (atomic orbital), OAO (orthogonalized atomic orbital), HAO (hybrid atomic orbitals) and OHAO (orthogonalized hybrid atomic orbitals) basis sets, and the "valence orbital" approximation. Numerical results indicate that the common approximations of "semi-empirical valence electron methods" known as "diatomic", "intermediate" and "complete" neglect of differential overlap are best justified for OHAO sets (and to a lesser extent for OAO sets). In the following chapter the author presents his ideas on methods for calculating molecular integrals. The final chapters are devoted to methods "beyond the MO method" (VB and CI), and to applications to polymers, solids, and inorganic molecules.

In my opinion, the most readable and valuable chapters (for chemists) are those on the orbital transformations and on polymers and solids.

In his preface the author states: "This book represents an approach to the theory of molecular electronic structure by treating valence and qualitative features of electronic structure as being of interest *per se* and not merely "disposables" on the path to numerical results". Accordingly, this is not a book written for experimentalists who like to have methods that produce numbers to be compared to their measured data and who want to know about the effectiveness of the various "semi-empirical" procedures available to generate these numbers. In my opinion, this is also not a book that could serve as a textbook for beginners or students to be introduced to molecular orbital theories or even to "semi-empirical" valence electron methods. This book is for quantum chemists and will be most profitable to those who have some interest and experience in the field of valence electron methods.

Armin Schweig, Marburg

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