Theoret. Chim. Acta (Berl.) 47, 81–82 (1978)

THEORETICA CHIMICA ACTA

Book Reviews

B. Pullman, R. G. Parr (Eds.): The New World of Quantum Chemistry. Dordrecht (Holland) and Boston (USA): D. Reidel Publishing Co. 1976. VIII + 356 pp., price: Dfl. 75,–/US $29.00

This book collects the lectures of the Second International Congress of Quantum Chemistry held at New Orleans, USA, in 1976, just as a preceding volume collected those of the first Congress (see Theoret. Chim. Acta (Berl.) **40**, 349 (1975)). However, there is a subtle difference in the titles of both volumes. While the first book was entitled "The World . . .", this new volume has been entitled "The New World . . .". In effect, the latter title points to the fact that lectures on the new frontiers of Quantum Chemistry in the fields of Biochemistry, Pharmacology, Environmental Effects, and Surface Chemistry and Catalysis, which have provided such promising results so far, are included.

The topics covered by these lectures include not only the already classical ones in quantum chemistry although treated with new methodology (for, as Professor Hirschfelder has well said, "Like 90% of all the academic scientists, I still work on the problems considered in my doctor's thesis"), but also the foremost fronts of today's quantum chemistry as we pointed out before. That is, they include the wide spectrum of topics which, with words of Professor Hirschfelder himself, correspond to the so-called *Platinum Age of Quantum Chemistry*.

Since the lectures are in general developed by well-known specialists in the various areas, they mainly reflect the investigations and perspectives of the authors themselves. Their lectures will be of great utility to all quantum chemists as well as to those interested in the recent developments of quantum chemistry even though the latter may have some difficulty in reading some of these topics.

The lectures are collected in the following symposia:

Symposium I. Foundations of Quantum Chemistry

- Present Status of the Correlation Problem (R. McWeeny, pp. 3–31).
  Excellent summary of the progress made in this field in the last ten years.
- Quantum Mechanical Facets of Chemical Bonds (R. Daudel, pp. 33–56).
  Interesting study of the energetic, density, partitioning, and functional aspects of the chemical bond.
- Propagator Theory of Atomic and Molecular Structure (Y. Öhrn, pp. 57–78).
  A general exposition is made of the methods without wavefunctions, followed by a thorough development of propagator theory.

Symposium II. Molecular Scattering

- Quantized Vortices in Molecular Scattering (J. O. Hirschfelder, pp. 81–86).
  This theory is applied to the study of idealized models: sphere–sphere elastic scattering and reactive collinear atom–diatomic molecule collision.
- Recent Developments in Semiclassical Mechanics: Eigen Values and Reaction Rate Constants (W. H. Miller, pp. 87–102).
  A semiclassical treatment of eigenvalues for a multidimensional potential well and of the rate constant for a chemical reaction with an activation barrier is presented.
- Energy Consumption and Energy Disposal in Elementary Chemical Reactions (R. D. Levine, pp. 103–129).
  A very thorough analysis of the specificity of internal energy disposal and of the selectivity of internal energy consumption in elementary chemical reactions is made.

Symposium III. Quantum Organic Chemistry and beyond

- Introduction (B. Pullman, pp. 133–135).

- Computational Methods for Large Molecules (G. G. Hall, pp. 137–187).
  A general introduction and an evaluation of the methods used in the study of these systems are presented.

- The Solvent Effect: Recent Developments (A. Pullman, pp. 149–187).
  This is a very thorough study of one of the most recent exploring fields of quantum chemistry in which environmental effects are considered in computations of molecular structures and properties, including solvent effects and cation and counterion binding.

- Quantum Pharmacology (R. E. Christoffersen, pp. 189–210).
  It deals with very recent quantum mechanical studies on drug design and the current activities and future direction in the field.

Symposium IV. Potential Surfaces, Transition States, and Intermediates in Chemical and Photochemical Processes

- Calculation of Potential Surface for Ground and Excited States (S. D. Peyerimhoff and R. I. Buenker, pp. 213–240).
  This is a profound and interesting study of the applications of the different types of *ab initio* calculations in the determination of potential energy surfaces, which shows that use of multiconfigurational techniques are essential in the treatment of chemical problems specially when excited states are involved.

- Transition States and Reaction Mechanisms in Organic Chemistry (L. Salem, pp. 241–269).
  This is a very thorough analysis of the description of the transition state (more appropriately called transition "structure" as the author suggests?), of the determination of the potential energy surfaces using electronic control by orbital symmetry and by state symmetry, and its application to photochemical reactions.

Symposium V. Surface Quantum Chemistry and Catalysis

- Introductory Remarks on the Quantum Theory of Catalysis and Related Surface Phenomena (K. Fukui, pp. 273–277).
  This is a brief introduction to the study of the catalytic activity of transition metals which includes size of the system concerned, orbital interaction in catalysis, and origin of catalytic activity.

- Methods for Surface Quantum Chemistry (J. Koutecký, pp. 279–303).
  After a survey of different approaches in order to describe the chemical properties of solids, the author develops the one-electron approximation to surface states and applies the Green operators to the theory of surface states and chemisorption.

- The Chemisorption Bond (J. R. Schrieffer, pp. 305–315).
  Since to describe the chemisorption bond basic concepts of quantum mechanics and solid state theory are needed, the author deals with the study of one-electron schemes, bond locality, effective potential, excitations, and limitations of the local density approximation.

- Molecular Clusters and Catalytic Activity (K. H. Johnson, pp. 317–356).
  This is a valuable and extensive study of the application of the self-consistent field-Xα-scattered wave (SCF-Xα-SW) method to the study of transition and noble metal clusters, bimetallic clusters and the effects of alloying, magnetic effects in metallic and bimetallic clusters, effects of the supporting environment, iron-sulfur proteins, and chemisorption and reactivity on metallic clusters.

There exist some typographical errors which, however, the reader may easily verify.

J. J. Fernández-Alonso

Received July 26, 1977

Theoret. Chim. Acta (Berl.) 47, 83 (1978)

THEORETICA CHIMICA ACTA

G. H. Wagnière: Introduction to Elementary Molecular Orbital Theory and to Semiempirical Methods. Lecture Notes in Chemistry, Vol. 1. Berlin: Springer-Verlag 1976, 109 pp., price DM 14,80 (US $6.10)

This booklet is the first in the series "Lecture Notes in Chemistry" which is edited by a group of scientists who are known from their work in physical and theoretical chemistry. According to the publishers' intention this series aims "to report new developments in chemical research and teaching". Preliminary drafts, lectures, seminar work-outs and reports on meetings are planned to be published quickly, informally and at a high level.

Accordingly, the present volume summarizes lectures held by the author on various occasions; it is a well presented and carefully chosen collection of formulas supplemented by a text which concisely explains the symbols, however, not much going into details on their physical implications. Therefore, the book should address people who know already some fundamental wave mechanics and want to get some experience in computing procedures.

Following the hierarchy of approximations the author removes from the most general formula, via Born–Oppenheimer, the nuclear motion, splits up the number of electrons into different groups, and treats the π-electrons either by Hückel or by more advanced semiempirical methods without or with including configuration interaction by which all difficulties arise connected with the two-electron problem. The treatment becomes even more formalistic when the SCF methods for closed and open shell systems are presented adding some of their numerous semiempirical simplifications necessarily to be made when calculating larger systems. These procedures are applied in particular when only valence electrons are considered, however, leading to some fundamental difficulties arising from a dependence of model parameters on the orbital basis. The final chapter contains some special topics among which the treatment of the Cotton effect must be emphasized where expressions for the rotatory strength are given which usually are not found in a volume of this size. The consideration of three examples demonstrates the usefulness of the presented formulas finally reconciling those readers who are perhaps expecting to find more chemistry rather than formalism in this book.

I believe that this booklet is useful for everybody who wants to apply MO procedures to his own problems, as well as for those who just look for a compact compilation.

H.-H. Schmidtke

Received September 14, 1977