By ERICH STEINER

Department of Chemistry, University of Exeter, Exeter

With the advent during the past few years, and the continuing development, of large high-speed computers which are efficient data-processing machines, there has been a renewed interest in the non-empirical computation of accurate wave functions for chemically non-trivial systems. Although there have been several important and interesting developments in theory and method, such as in the application of density matrix theory and of many-body techniques to quantum chemistry, we shall confine our attention here to a review of the recent non-empirical applications of molecular orbital theory to the prediction and interpretation of the shapes and properties of polyatomic molecules and, in particular, to the use of Gaussian functions in the calculation of the orbitals. No attempt is made to give a complete and comprehensive survey of the work published during any recent period, but rather to use the literature to illustrate some of the methods, problems, and achievements of molecular orbital theory.

1 Non-empirical Theories

By a non-empirical (or ab initio) theory in molecular quantum chemistry is meant the solution of a time-independent Schrödinger equation

$$\mathscr{H} \Psi = E \Psi$$
 (1)

in which the Hamiltonian \mathscr{H} is that appropriate for any model of the system which does not, either explicitly or implicitly, depend on the properties of any finite number of the states of the system.

The simplest and most commonly used model of a molecule involves the following assumptions:

- (i) The nuclei and electrons are treated as point charges.
- (ii) Only the electrostatic (Coulomb) interactions are considered in the first place, and the force between charges q_1 and q_2 separated by distance r is $q_1q_2/4\pi\epsilon_0r^2$, where ϵ_0 is the permittivity of a vacuum.
- ¹ 'Reduced Density Matrices with Applications to Physical and Chemical Systems', eds., A. J. Coleman and R. M. Erdahl, Queen's Papers on Pure and Applied Mathematics—No. 11, Queen's University, Kingston, Ontario, 1968.
- Correlation Effects in Atoms and Molecules', eds., R. Lefebvre and C. Moser, Adv. Chem. Phys., 1969, 14.

Determination And Interpretation Of Molecular Wave Functions

Rachel Sandford

Determination And Interpretation Of Molecular Wave Functions:

The Determination and Interpretation of Molecular Wave Functions Erich Steiner,1976-07-15 First published in 1976 this monograph presents an exposition of some of the more important theoretical and computational techniques that have been developed for the determination and interpretation of molecular wave functions Although a comprehensive theory of the electronic structure and bonding in molecules had been developed by 1960 only with the advent of the electronic computer in the late 1950s did it become possible to perform accurate non empirical calculations for molecules of chemical interest indeed much of the subsequent evolution of the theory has occurred in parallel with the development of computing machines and techniques

Chemické Zvesti ,1976 Molecular Wave Functions ,1969 Scientific and Technical Aerospace Reports ,1975

Spectroscopia Molecular ,1977 Canadian Journal of Chemistry ,2003

Theoretical Chemistry Amyand David Buckingham, Charles Alfred Coulson, 1975 Molecular charge distributions their display and use correlated wave functions obtcuned by the variational nethod and the method of moments Electron momentum distribution in atoms molecules and solids Electronic structure of small molecules ESCA chemical bonding aspects of some solid state phenomena The SCF Xa scat tered ware method and its application to molecular problems The theory of rotationally inelastic molecular collisions Radiationless transitions The Development of Theoretical and He(I) Photoelectron Methods for the Determination and Interpretation of the Electronic Structure of Large Molecules Dennis Lee Lichtenberger, 1974 Nuclear Science Abstracts, 1975 Advanced Quantum Chemistry Hendrik F. Hameka, 1965

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Sci-tech Book Profiles, 1965 Includes title page table of contents list of contributors preface and all indexes of each book

Infra-red Analysis of Molecular Structure
Technical Books and Serials in Print ,1984

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Chemical Explanation Joseph E. Earley,2003 Over many centuries chemists and their alchemical predecessors evolved a sophisticated array of concepts and methods that yield reliable understanding when applied to systems of complexity intermediate between those generally considered by physicists at one extreme and biologists at the other Chemical problems can be chosen so that quantitative modelling can be used fruitfully while also displaying some of the intriguing features typical of more complex cases Papers in this volume address relations between macroscopic and microscopic descripion essential roles of visualization and representation in chemical understanding historical questions involving chemical concepts impacts of chemical ideas on wider cultural concerns and relationships between contemporary chemistry and other sciences The authors demonstrate assert or tacitly assume that chemical explanation is functionally autonomous This volume should be of interest not only to professional chmists and

philosophers but also to workers in medicine psychology and other fields in which relationships between explanations based on diverse levels of description and investigation are important

Journal of the Chemical Society ,1973

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