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Semiempirical Methods Of Electronic Structure Calculation Part A Techniques Modern Theoretical Chemistry 7

Robert S. Mulliken

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fact that no approximations are involved in the evaluation of the required molecular integrals Consistent with current activity in the field the first of these two volumes contains chapters dealing with methods per se while the second concerns the application of these methods to problems of chemical interest In asense the motivation for these volumes has been the spectacular recent success of ab initio theory in resolving important chemical questions However these applications have only become possible through the less visible but equally important efforts of those developing new theoretical and computational methods and models Henry F Schaefer VII Contents Contents of Volume 4 XIX Chapter 1 Gaussian Basis Sets for Molecular Calculations Thom H Dunning Ir and P Ieffrey Hay 1 Introduction 1 1 1 Slater Functions and the Hydrogen Moleeule 1 1 2 Gaussian Functions and the Hydrogen Atom 3 2 Hartree Fock Calculations on the First Row Atoms 5 2 1 Valence States of the First Row Atoms 6 7 2 2 Rydberg States of the First Row Atoms 9 2 3 Theoretical Treatment of Large Molecules and Their Interactions Zvonimir B. Maksic, 2013-03-07 The French chemist Marcelin Berthelot put forward a classical and by now an often cited sentence revealing the quintessence of the chemical science La Chimie cree son objet This is certainly true because the largest number of molecular compounds were and are continuously synthesized by chemists themselves However modern computational quantum chemistry has reached a state of maturity that one can safely say La Chimie Theorique cree son objet as well Indeed modern theoretical chemistry is able today to provide reliable results on elusive systems such as short living species reactive intermediates and molecules which will perhaps never be synthesized because of one or another type of instability It is capable of yielding precious information on the nature of the transition states reaction paths etc Additionally computational chemistry gives some details of the electronic and geometric structure of molecules which remain hidden in experimental examinations Hence it follows that powerful numerical techniques have substantially enlarged the domain of classical chemistry. On the other hand interpretive quantum chemistry has provided a conceptual framework which enabled rationalization and understanding of the precise data offered either by experiment or theory It is modelling which gives a penetrating insight into the chemical phenomena and provides order in raw experimental Polyatomic Molecules Robert S. results which would otherwise represent just a large catalogue of unrelated facts Mulliken, 2012-12-02 Polyatomic Molecules Results of Ab Initio Calculations describes the symmetry of polyatomic molecules in ground states This book contains 12 chapters that also cover the excited and ionized states of these molecules The opening chapter describes the nature of the various ab initio computational methods. The subsequent four chapters deal with the three atom systems differing with respect to the number of hydrogen atoms in the molecules These chapters also discuss the reaction surfaces of these systems These topics are followed by discussions on the molecules whose ground states belong to relatively high little or no symmetry groups The concluding chapters explore the inorganic and relatively large organic molecules These chapters also examine the ab initio calculations of molecular compounds and complexes as well as hydrogen bonding and ion hydration This text will be of great value to organic and inorganic chemists and physicists Chemical

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