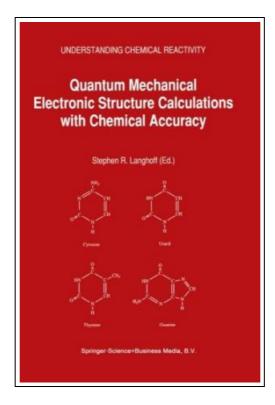
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Book Condition: New. Publisher/Verlag: Springer Netherlands | The theoretical chemist is accustomed to judging the success of a theoretical prediction according to how well it agrees with an experimental measurement. Since the object of theory is the prediction of the results of experiment, that would appear to be an entirely satisfactory state ofaffairs. However, ifit is true that "the underlying physicallaws . for the whole ofchemistryare . completely known" (1), thenit shouldbepossible,atleastinprinciple, topredict theresults of experiment moreaccurately than they canbe measured. If the theoreticalchemist could obtain exact solutions of the Schrodinger equation for many-body systems, then the experimental chemist would soon become accustomed to judging the success of an experimental measurement by how well it agrees with a theoretical prediction. In fact, it is now possible to obtainexact solutions of the Schrodinger equation for systems of a few electrons(2-8). These systems include the molecular ion Ht, the molecule H , the reaction intermediate H-H-H, the unstable pair H-He, the 2 stable dimer He2' and the trimer He3. The quantum Monte Carlo method used in solving the time-independent Schrodinger equation for these systems is exact in that it requires no physical or mathematical assumptions beyond those of the Schrodinger equation. As in most Monte Carlo methods there is a statistical or sampling error which is readily estimated. | Exact Quantum Chemistry by Monte Carlo Methods; J.B. Anderson. Achieving Chemical Accuracy with Coupled-Cluster Theory; T.J. Lee, G.E. Scuseria. Magnetic Hyperfine Coupling Constants in Free Radicals; D.M. Chipman. Calculation of Accurate Bond Energies, Electron Affinities, and Ionization Energies; L.A. Curtiss, K. Raghavachari. Accurate Theoretical Studies of Small Elemental Clusters; K. Raghavachari, L.A. Curtiss. Electronic Spectroscopy of Diatomic Molecules; H. Partridge, S.R. Langhoff, C.W. Bauschlichter Jr. Theoretical Spectroscopy of Small Molecules: Ab Initio Inves

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