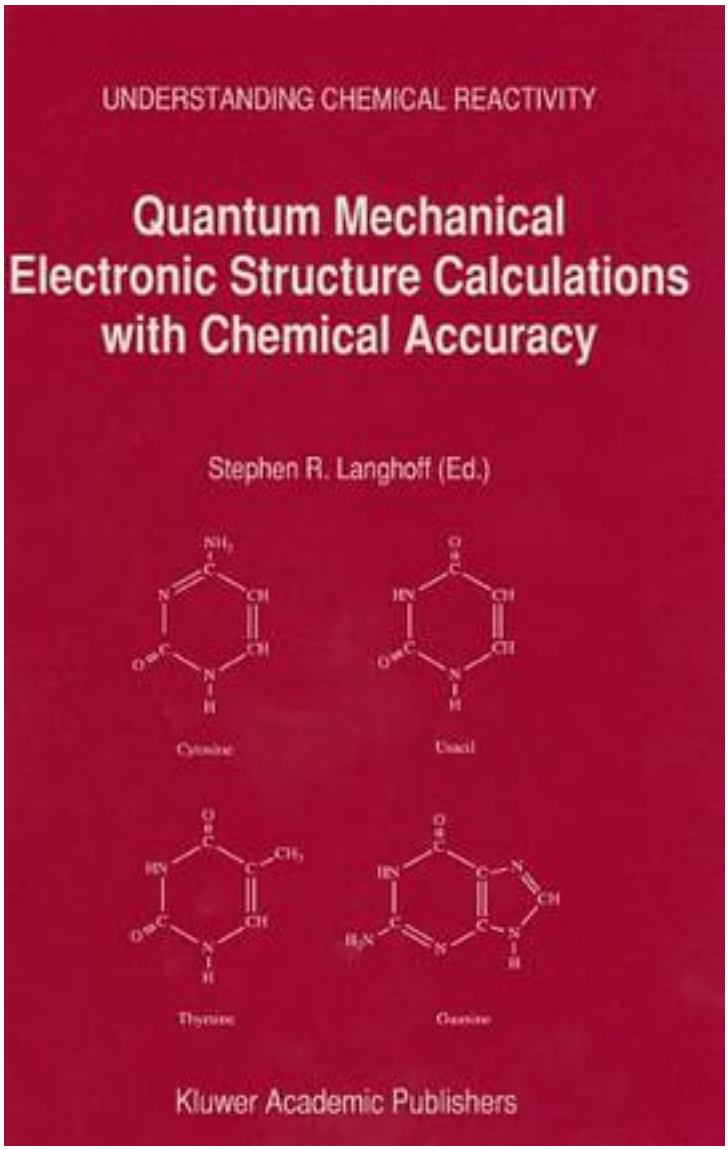
Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy



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The principal focus of this volume is to illustrate the level of accuracy currently achievable by "ab initio" quantum chemical calculations. While new developments in theory are discussed to some extent, the major emphasis is on a comparison of calculated properties with experiments. This focus is similar to the one taken in the book, "Comparison of Ab Initio Quantum Chemistry with Experiment for Small Molecules", edited by Rodney Bartlett (Reidel, 1984). However, the phenomenal improvement in both theoretical methods and computer architecture have made it possible to obtain accurate results for rather large molecular systems. For example, the electronic spectra of the nucleic acid base monomer structures shown on the front cover have been obtained using a fully correlated "ab initio" study. This text is intended for researchers, teachers and students in chemistry and physics.

作者介绍:

目录:

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