

# Quantum-Mechanical Prediction of Thermochemical Data

2007, Overman, (Ed.)



# Quantummechanical Prediction Of Thermochemical Data

**Edward I. Solomon, Robert A. Scott, R.  
Bruce King**



## **Quantummechanical Prediction Of Thermochemical Data:**

*Quantum-Mechanical Prediction of Thermochemical Data* Jerzy Cioslowski, 2006-04-11 For the first time in the history of chemical sciences theoretical predictions have achieved the level of reliability that allows them to validate experimental measurements in accuracy on a routine basis Only a decade ago such a statement would be valid only with severe qualifications as high level quantum chemical calculations were feasible only for molecules composed of a few atoms Improvements in both hardware performance and the level of sophistication of electronic structure methods have contributed equally to this impressive progress that has taken place only recently The contemporary chemist interested in predicting thermochemical properties such as the standard enthalpy of formation has at his disposal a wide selection of theoretical approaches differing in the range of applicability computational cost and the expected accuracy Ranging from high level treatments of electron correlation used in conjunction with extrapolative schemes to semiempirical methods these approaches have well known advantages and shortcomings that determine their usefulness in studies of particular types of chemical species The growing number of published computational schemes and their variants testing sets and performance statistics often makes it difficult for a scientist not well versed in the language of quantum theory to identify the method most adequate for his research needs

**Quantum-Mechanical Prediction of Thermochemical Data** Department of Theoretical Chemistry Jerzy Cioslowski, 2014-01-15 The contemporary chemist interested in predicting thermochemical properties such as the standard enthalpy of formation has at his disposal a wide selection of theoretical approaches differing in the range of applicability computational cost and the expected accuracy Ranging from high level treatments of electron correlation used in conjunction with extrapolative schemes to semiempirical methods these approaches have well known advantages and shortcomings that determine their usefulness in study of particular types of chemical species The growing number of published computational schemes and their variants testing sets and performance statistics often makes it difficult for a scientist not well versed in the language of quantum theory to identify the method most adequate for his research needs In this book the experts who have developed and tested many of the currently used electronic structure procedures present an authoritative overview of the tools for the computation of thermochemical properties of atoms and molecules Theory and Applications of Computational Chemistry Clifford Dykstra, Gernot Frenking, Kwang Kim, Gustavo Scuseria, 2011-10-13 Computational chemistry is a means of applying theoretical ideas using computers and a set of techniques for investigating chemical problems within which common questions vary from molecular geometry to the physical properties of substances Theory and Applications of Computational Chemistry The First Forty Years is a collection of articles on the emergence of computational chemistry It shows the enormous breadth of theoretical and computational chemistry today and establishes how theory and computation have become increasingly linked as methodologies and technologies have advanced Written by the pioneers in the field the book presents historical perspectives and insights into the subject and addresses new and current methods as

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Computational Inorganic and Bioinorganic Chemistry Edward I. Solomon, Robert A. Scott, R. Bruce King, 2013-02-19 Over the past several decades there have been major advances in our ability to computationally evaluate the electronic structure of inorganic molecules particularly transition metal systems This advancement is due to the Moore's Law increase in computing power as well as the impact of density functional theory DFT and its implementation in commercial and freeware programs for quantum chemical calculations Improved pure and hybrid density functionals are allowing DFT calculations with accuracy comparable to high level Hartree Fock treatments and the results of these calculations can now be evaluated by experiment When calculations are correlated to and supported by experimental data they can provide fundamental insight into electronic structure and its contributions to physical properties and chemical reactivity This interplay continues to

expand and contributes to both improved value of experimental results and improved accuracy of computational predictions. The purpose of this EIC Book is to provide state of the art presentations of quantum mechanical and related methods and their applications written by many of the leaders in the field. Part 1 of this volume focuses on methods their background and implementation and their use in describing bonding properties energies transition states and spectroscopic features. Part 2 focuses on applications in bioinorganic chemistry and Part 3 discusses inorganic chemistry where electronic structure calculations have already had a major impact. This addition to the EIC Book series is of significant value to both experimentalists and theoreticians and we anticipate that it will stimulate both further development of the methodology and its applications in the many interdisciplinary fields that comprise modern inorganic and bioinorganic chemistry. This volume is also available as part of Encyclopedia of Inorganic Chemistry 5 Volume Set. This set combines all volumes published as EIC Books from 2007 to 2010 representing areas of key developments in the field of inorganic chemistry published in the Encyclopedia of Inorganic Chemistry. Find out more

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Wilson, 2007 Modeling is becoming a significant component in the design and analysis of chemical systems in areas such as catalysis nanomaterials and biological systems With rapidly advancing technology there is an increasing need to model molecules that are quite large and complex and to model such systems with reasonable accuracy However computational methods are generally more numerous and reliable for lighter smaller molecules since calculations on smaller molecules are less computationally demanding than for larger molecules and can take advantage of high accuracy but prohibitively expensive computational approaches Two widely used approaches for chemical modeling are ab initio correlated methods and density functional theory Though there is great interest in using these methods for high accuracy calculations on increasingly larger and more complex chemical systems each approach currently has limitations Ab initio methods suffer from a high N scaling problem where the N scaling represents the computational cost memory disk space and time requirements of the calculations thus making high accuracy calculations Density functional methods have a much lower N scaling and thus calculations can be done on much larger molecules Unfortunately density functional calculations are generally not as reliable as ab initio approaches and sometimes at best can only provide a qualitative description of properties of interest This volume brings together researchers from throughout the world to assess recent progress in the field of electronic structure methodology focusing upon ab initio and density functional developments and to discuss future direction This publication will impact a number of fields including computational chemistry organic chemistry and inorganic chemistry It will help to provide a closer commonality of ab initio and density functional approaches as it brings together many of the top senior and junior scientists in both fields to address a common problem high accuracy modeling of larger chemical systems



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