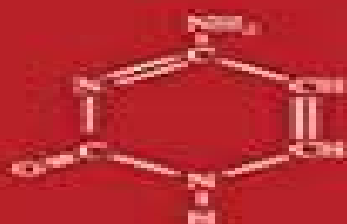


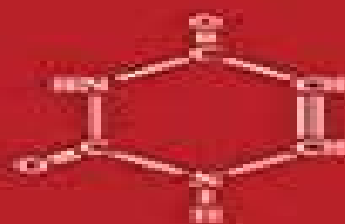
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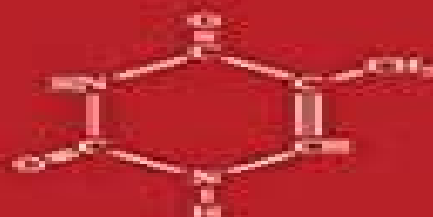
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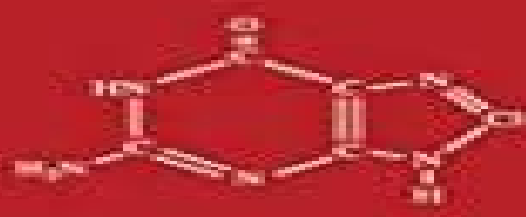
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Molecular Electronic-Structure Theory Trygve Helgaker, Poul Jorgensen, Jeppe Olsen, 2014-08-11 Ab initio quantum chemistry has emerged as an important tool in chemical research and is applied to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum mechanical methods. This is the first comprehensive up to date and technical work to cover all the important aspects of modern molecular electronic structure theory. Topics covered in the book include: Second quantization with spin adaptation, Gaussian basis sets and molecular integral evaluation, Hartree Fock theory, Configuration interaction and multi configurational self consistent theory, Coupled cluster theory for ground and excited states, Perturbation theory for single and multi configurational states, Linear scaling techniques and the fast multipole method, Explicitly correlated wave functions, Basis set convergence and extrapolation, Calibration and benchmarking of computational methods with applications to molecular equilibrium structure, atomization energies and reaction enthalpies. *Molecular Electronic Structure Theory* makes extensive use of numerical examples designed to illustrate the strengths and weaknesses of each method treated. In addition statements about the usefulness and deficiencies of the various methods are supported by actual examples not just model calculations. Problems and exercises are provided at the end of each chapter complete with hints and solutions. This book is a must for researchers in the field of quantum chemistry as well as for nonspecialists who wish to acquire a thorough understanding of ab initio molecular electronic structure theory and its applications to problems in chemistry and physics. It is also highly recommended for the teaching of graduates and advanced undergraduates. New Methods in Computational Quantum Mechanics Ilya Prigogine, Stuart A. Rice, 2009-09-09 The use of quantum chemistry for the quantitative prediction of molecular properties has long been frustrated by the technical difficulty of carrying out the needed computations. In the last decade there have been substantial advances in the formalism and computer hardware.

needed to carry out accurate calculations of molecular properties efficiently These advances have been sufficient to make quantum chemical calculations a reliable tool for the quantitative interpretation of chemical phenomena and a guide to laboratory experiments However the success of these recent developments in computational quantum chemistry is not well known outside the community of practitioners In order to make the larger community of chemical physicists aware of the current state of the subject this self contained volume of Advances in Chemical Physics surveys a number of the recent accomplishments in computational quantum chemistry This stand alone work presents the cutting edge of research in computational quantum mechanics Supplemented with more than 150 illustrations it provides evaluations of a broad range of methods including Quantum Monte Carlo methods in chemistry Monte Carlo methods for real time path integration The Redfield equation in condensed phase quantum dynamics Path integral centroid methods in quantum statistical mechanics and dynamics Multiconfigurational perturbation theory applications in electronic spectroscopy Electronic structure calculations for molecules containing transition metals And more Contributors to New Methods in Computational Quantum Mechanics KERSTIN ANDERSSON Department of Theoretical Chemistry Chemical Center Sweden DAVID M CEPERLEY National Center for Supercomputing Applications and Department of Physics University of Illinois at Urbana Champaign Illinois MICHAEL A COLLINS Research School of Chemistry Australian National University Canberra Australia REINHOLD EGGER Fakultät für Physik Universität Freiburg Freiburg Germany ANTHONY K FELTS Department of Chemistry Columbia University New York RICHARD A FRIESNER Department of Chemistry Columbia University New York MARKUS P F LSCHER Department of Theoretical Chemistry Chemical Center Sweden K M HO Ames Laboratory and Department of Physics Iowa State University Ames Iowa C H MAK Department of Chemistry University of Southern California Los Angeles California PER KE Malmqvist Department of Theoretical Chemistry Chemical Center Sweden MANUELA MERCHÁN Departamento de Química Física Universidad de Valencia Spain LUBOS MITAS National Center for Supercomputing Applications and Materials Research Laboratory University of Illinois at Urbana Champaign Illinois STEFANO OSS Dipartimento di Fisica Università di Trento and Istituto Nazionale di Fisica della Materia Unit di Trento Italy KRISTINE PIERLOOT Department of Chemistry University of Leuven Belgium W THOMAS POLLARD Department of Chemistry Columbia University New York BJ RN O ROOS Department of Theoretical Chemistry Chemical Center Sweden LUIS SERRANO ANDRÁS Department of Theoretical Chemistry Chemical Center Sweden PER E M SIEGBAHN Department of Physics University of Stockholm Stockholm Sweden WALTER THIEL Institut für Organische Chemie Universität Zürich Zürich Switzerland GREGORY A VOTH Department of Chemistry University of Pennsylvania Pennsylvania C Z Wang Ames Laboratory and Department of Physics

Accurate Structure Determination of Free Molecules Jean Demaison, Natalja Vogt, 2020-12-02 This book presents a detailed look at experimental and computational techniques for accurate structure determination of free molecules The most fundamental property of a molecule is its structure it is a prerequisite for determining and understanding most other important properties

of molecules The determination of accurate structures is hampered by a myriad of factors subjecting the collected data to non negligible systematic errors This book explains the origin of these errors and how to mitigate and even avoid them altogether It features a detailed comparison of the different experimental and computation methods explaining their interplay and the advantages of their combined use Armed with this information the reader will be able to choose the appropriate methods to determine to a great degree of accuracy the relevant molecular structure

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Ruoff,2000-07-06 *Fullerenes* a guide to the current state of knowledge in the field The last decade has seen an explosion of research into the chemical and physical properties of a promising new class of carbon based materials known as fullerenes Karl Kadish and Rodney Ruoff two highly recognized leaders in the fullerene and nanotube research community edit a comprehensive and much needed survey of this important and rapidly evolving field Contributions by experts in diverse areas of chemistry physics pharmacology materials science and chemical engineering provide an excellent introduction to fullerenes and highlight their considerable potential in such cutting edge applications as semiconductor materials new pharmaceutical compounds and polymers From the electrochemistry of fullerenes to molecular and solid C₃₆ this book offers a remarkably fresh and authoritative look at some of the hottest research topics today including Organic functionalization of fullerenes Photophysical properties of different types of fullerenes Polyfunctional polymer derivatives of fullerenes The theory and production of endohedral metallofullerenes Fullerene surface interactions Superconductivity in fullerenes Synthesis of materials incorporated within carbon nanotubes *Advanced Topics in Theoretical Chemical Physics* Jean Maruani,Roland Lefebvre,Erkki J. Brändas,2003-11-30 *Advanced Topics in Theoretical Chemical Physics* is a collection of 20 selected papers from the scientific presentations of the Fourth Congress of the International Society for Theoretical Chemical Physics ISTCP held at Marly le Roi France in July 2002 *Advanced Topics in Theoretical Chemical Physics* encompasses a broad spectrum in which scientists place special emphasis on theoretical methods in chemistry and physics The chapters in the book are divided into five sections I Advances Chemical Thermodynamics II Electronic Structure of Molecular Systems III Molecular Interaction and Dynamics IV Condensed Matter V Playing with Numbers This book is an invaluable resource for all

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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 well as problems and applications in theoretical and computational chemistry Easy to read and packed with personal insights technical and classical information this book provides the perfect introduction for graduate students beginning research in this area It also provides very readable and useful reviews for theoretical chemists Written by well known leading experts Combines history personal accounts and theory to explain much of the field of theoretical and computational chemistry Is the perfect introduction to the field

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hydrogen bonded molecules and our understanding of their role in the atmospheric processes an ensemble of related topics are covered by a team of expert co authors The general properties of the weakly bound molecular complexes or clusters are discussed as well as their distribution in the planetary atmospheres Collision induced and dimeric absorption and emission are considered in the context of atmospheric spectroscopy The advanced experimental techniques which enable us to study the spectroscopic features of molecular complexes in the gas phase or which are adsorbed are reviewed The role of molecular complexes in the cometary atmosphere the Earth mesosphere and the atmospheres of the giant planets and some of their satellites are also discussed in detail

Molecular Modelling and Drug Design K Anand Solomon, 2019-06-05

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