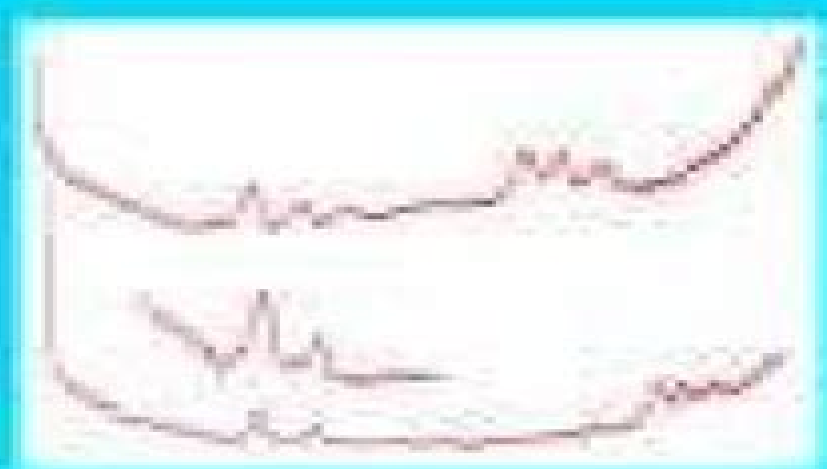


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Equilibrium Structural Parameters

István Hargittai, M. Hargittai



Equilibrium Structural Parameters:

Equilibrium Structural Parameters, 1999-11-30 The current volume in the series *Vibrational Spectra and Structure* is a single topic volume on gas phase structural parameters The title of the volume *Equilibrium Structural Parameters* covers the two most common techniques for obtaining gas phase structural parameters microwave spectroscopy and the electron diffraction technique Since the quantum chemical method provides equilibrium geometries the volume is an attempt to provide a connection between the experimental and theoretical parameters The book provides a review on molecular structure determinations from spectroscopic data using scaled moments of inertia The limited number of molecules for which equilibrium parameters have been obtained and the requirement of a large number of microwave data needed to obtain the equilibrium structural parameters is noted Electron diffraction technique is reviewed along with a description of how this can incorporate structural information from microwave spectroscopy vibrational spectroscopy or theoretical calculations to improve the determination of the structural parameters by electron diffraction studies Also discussed are the theory and methods of microwave spectroscopy describing in some detail r_0 and r_s structures as well as r_m structures and corrections based on ab initio calculations The accuracy of the molecular geometry predictions by quantum chemical methods is considered in some detail with data presented in graphic rather than tabular form This makes it possible to readily note the difference in the parameters predicted at the various levels of quantum mechanical calculations The four authors have provided a coherent description of the various structural parameters obtained experimentally along with treatments needed to extract equilibrium bond distances and angles *Thermodynamic Properties of Solids* S. L. Chaplot, R. Mittal, N.

Choudhury, 2010-02-19 Recent years have seen a growing interest in the field of thermodynamic properties of solids due to the development of advanced experimental and modeling tools Predicting structural phase transitions and thermodynamic properties find important applications in condensed matter and materials science research as well as in interdisciplinary research involving geophysics and Earth Sciences The present edited book with contributions from leading researchers around the world is aimed to meet the need of academic and industrial researchers graduate students and non specialists working in these fields The book covers various experimental and theoretical techniques relevant to the subject **The Atom-Atom Potential Method** Alexander J. Pertsin, Alexander I. Kitaigorodsky, 2012-12-06 The history of physics furnishes many examples of how a simple semiempirical method essentially based on intuitive considerations may prove to be much more successful than a rigorous theoretical approach A pertinent example is the method of atom atom potentials which treats the intermolecular interactions between polyatomic molecules in terms of pairwise interactions between their constituent atoms Despite a few conceptual shortcomings the method provides a fairly reliable practical means of handling on a microscopic level a wide range of problems that arise in the solid state physics and chemistry of organic compounds This monograph is an attempt to generalize the experience gained in the past twenty years in interpreting the static and dynamic

properties of organic molecular solids in terms of atom atom potentials It embraces nearly all aspects of the application of the method including an evaluation of cohesive energies equilibrium crystal structures phonon spectra thermodynamic functions and crystal defects Many related topics such as the effect of the crystal field on molecular conformation the determination of crystal structures from raw diffraction data and the problem of polymorphic transitions are also discussed We believe that this book will be of use to researchers in solid state physics chemistry crystallography physical chemistry and polymer chemistry It also gives us an opportunity to acknowledge our indebtedness to those who sent us published as well as unpublished information and suggestions including A T Amos E L Bokhenkov H Bonadeo R K Boyd C P Multiphysics Modelling and Simulation for Systems Design and Monitoring Mohamed Haddar, Mohamed Slim Abbes, Jean-Yves Choley, Taoufik Boukharouba, Tamer Elnady, Andrei Kanaev, Mounir Ben Amar, Fakher Chaari, 2015-01-03 This book reports on the state of the art in the field of multiphysics systems It consists of accurately reviewed contributions to the MMSSD 2014 conference which was held from December 17 to 19 2004 in Hammamet Tunisia The different chapters covering new theories methods and a number of case studies provide readers with an up to date picture of multiphysics modeling and simulation They highlight the role played by high performance computing and newly available software in promoting the study of multiphysics coupling effects and show how these technologies can be practically implemented to bring about significant improvements in the field of design control and monitoring of machines In addition to providing a detailed description of the methods and their applications the book also identifies new research issues challenges and opportunities thus providing researchers and practitioners with both technical information to support their daily work and a new source of inspiration for their future research Handbook of High-resolution Spectroscopy Martin Quack, Frederic Merkt, 2011-09-26 The field of High Resolution Spectroscopy has been considerably extended and even redefined in some areas Combining the knowledge of spectroscopy laser technology chemical computation and experiments Handbook of High Resolution Spectroscopy provides a comprehensive survey of the whole field as it presents itself today with emphasis on the recent developments This essential handbook for advanced research students graduate students and researchers takes a systematic approach through the range of wavelengths and includes the latest advances in experiment and theory that will help and guide future applications The first comprehensive survey in high resolution molecular spectroscopy for over 15 years Brings together the knowledge of spectroscopy laser technology chemical computation and experiments Brings the reader up to date with the many advances that have been made in recent times Takes the reader through the range of wavelengths covering all possible techniques such as Microwave Spectroscopy Infrared Spectroscopy Raman Spectroscopy VIS UV and VUV Combines theoretical computational and experimental aspects Has numerous applications in a wide range of scientific domains Edited by two leaders in this field Provides an overview of rotational vibration electronic and photoelectron spectroscopy Volume 1 Introduction Fundamentals of Molecular Spectroscopy Volume 2 High Resolution Molecular

Spectroscopy Methods and Results Volume 3 Special Methods Applications **Molecular Spectroscopy**, 1962

Bioinformatics of Genome Regulation and Structure II Nikolay Kolchanov, Ralf Hofstaedt, Luciano Milanesi, 2006-06-15

The last 15 years in development of biology were marked with accumulation of unprecedentedly huge arrays of experimental data. The information was amassed with exclusively high rates due to the advent of highly efficient experimental technologies that provided for high throughput genomic sequencing of functional genomics technologies allowing investigation of expression dynamics of large groups of genes using expression DNA chips of proteomics methods giving the possibility to analyze protein compositions of cells, tissues and organs, assess the dynamics of the cell proteome and reconstruct the networks of protein-protein interactions and of metabolomics. In particular, high-resolution mass spectrometry study of cell metabolites and distribution of metabolic fluxes in the cells with a concurrent investigation of the dynamics of thousands of metabolites in an individual cell. Analysis, comprehension and use of the tremendous volumes of experimental data reflecting the intricate processes underlying the functioning of molecular genetic systems are unfeasible in principle without the systems approach and involvement of the state-of-the-art information and computer technologies and efficient mathematical methods for data analysis and simulation of biological systems and processes. The need in solving these problems initiated the birth of a new science: postgenomic bioinformatics or systems biology in silico. *Molecular Structure by Diffraction*

Methods G A Sim, L E Sutton, 2007-10-31 Specialist Periodical Reports provide systematic and detailed review coverage of progress in the major areas of chemical research. Written by experts in their specialist fields, the series creates a unique service for the active research chemist, supplying regular, critical, in-depth accounts of progress in particular areas of chemistry. For over 80 years the Royal Society of Chemistry and its predecessor the Chemical Society have been publishing reports charting developments in chemistry which originally took the form of Annual Reports. However, by 1967 the whole spectrum of chemistry could no longer be contained within one volume and the series Specialist Periodical Reports was born. The Annual Reports themselves still existed but were divided into two and subsequently three volumes covering Inorganic, Organic and Physical Chemistry. For more general coverage of the highlights in chemistry they remain a must. Since that time the SPR series has altered according to the fluctuating degree of activity in various fields of chemistry. Some titles have remained unchanged while others have altered their emphasis along with their titles; some have been combined under a new name whereas others have had to be discontinued. The current list of Specialist Periodical Reports can be seen on the inside flap of this volume. **Molecular Spectroscopy**

R F Barrow, Derek A Long, D J Millen, 2007-10-31 Specialist Periodical Reports provide systematic and detailed review coverage of progress in the major areas of chemical research. Written by experts in their specialist fields, the series creates a unique service for the active research chemist, supplying regular, critical, in-depth accounts of progress in particular areas of chemistry. For over 80 years the Royal Society of Chemistry and its predecessor the Chemical Society have been publishing reports charting developments in chemistry which originally took the

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Computations for the Nano-Scale P.E. Blöchl, C. Joachim, A.J. Fisher, 2012-12-06 Proceedings of the NATO Advanced Research Workshop Aspet France October 12 16 1992

CRC Concise Encyclopedia of Nanotechnology Boris Ildusovich Kharisov, Oxana Vasilievna Kharissova, Ubaldo Ortiz-Mendez, 2016-01-06 The CRC Concise Encyclopedia of Nanotechnology sets the standard against which all other references of this nature are measured As such it is a major resource for both skilled professionals and novices to nanotechnology The book examines the design application and utilization of devices techniques and technologies critical to research at the

Potential Energy Surfaces and Dynamics Calculations Donald Truhlar, 2013-11-11 The present volume is concerned with two of the central questions of chemical dynamics What do we know about the energies of interaction of atoms and molecules with each other and with solid surfaces How can such interaction energies be used to understand and make quantitative predictions about dynamical processes like scattering energy transfer and chemical reactions It is becoming clearly recognized that the computer is leading to rapid progress in answering these questions The computer allows probing dynamical mechanisms in fine detail and often allows us to answer questions that cannot be addressed with current experimental techniques As we enter the 1980 s not only are more powerful and faster computers being used but techniques and methods have been honed to a state where exciting and reliable data are being generated on a variety of systems at an unprecedented pace The present volume presents a collection of work that illustrates the capabilities and some of the successes of this kind of computer assisted research In a 1978 Chemical Society Report Frey and Walsh pointed out that it is extremely doubtful if a calculated energy of activation for any unimolecular decomposition can replace an experimental determination However they also recorded that they believed that some of the elaborate calculations being performed at present do suggest that we may be approaching a time when a choice between reaction mechanisms will be helped by such computational work

N Nitrogen Reinhard Haubold, Peter Merlet, Claudia Heinrich-Sterzel, Astrid Wietelmann, Ulrike Ohms-Bredeman, Carol Strametz, 2013-04-17 This volume deals with binary nitrogen hydrogen compounds having two three or more nitrogen atoms with the exception of hydrazine and with compounds composed of nitrogen hydrogen and noble gases The important species containing two nitrogen atoms N_2H N_2H^+ N_2H_2 and N_2H_3 are described in the first part of this volume Next chains and cycles consisting of three nitrogen atoms are covered Among them hydrogen

azide or hydrazoic acid HN_3 is the most extensively studied nitrogen hydrogen compound described in this volume With increasing number of nitrogen atoms the thermochemical stability declines There is however a considerable amount of information on molecules with up to nine linked nitrogen atoms Several of these binary nitrogen hydrogen compounds could only be isolated in the form of organic derivatives In that case data available for the organic derivatives were included if they were characteristic for the particular unsubstituted N H parent compound

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

Stereochemical Applications of Gas-Phase Electron Diffraction, Part A István Hargittai, M. Hargittai, 1988-10-01 Die erste umfassende Darstellung der Elektronenbeugung in der Gasphase einer sehr erfolgreichen Methode zur Bestimmung molekularer Geometrien Das Buch wendet sich in erster Linie an den Nicht Fachmann Die 26 Beiträge stammen von Autoren aus neun Ländern aus allen führenden auf diesem Gebiet arbeitenden Forschungslaboratorien Das Buch enthält einen einführenden Artikel von Herman Mark dem Pionier der Gasphasenelektronenbeugung und ein Vorwort von Jerome Karle dem Chemie Nobelpreisträger von 1985 Es wird nur zusammen in zwei Teilbänden abgegeben Teil A beschreibt Entwicklung und derzeitige Möglichkeiten der Methode darunter auch ihre Kombination mit anderen Verfahren Teil B enthält Ergebnisse von Strukturbestimmungen für zahlreiche Verbindungsklassen Er dient als umfassendes zuverlässiges Nachschlagewerk und bringt gleichzeitig Trends und Interpretationen von Strukturvariationen

Rheology of Paste in Metal Mines Aixiang Wu, 2022-04-01 This book investigates the rheology of paste in metal mines which is beneficial for cemented paste backfill CPB technology This book establishes a theory frame of paste rheology including measurement of the rheological properties of paste rheological behavior of full tailings in deep thickening rheological behavior of paste in the mixing process rheological behavior of paste in pipeline transportation and rheological behavior of filling body It aims to promote the development of paste theory the innovation of CPB technology and the research and development of CPB equipment to accelerate the construction of green mines based on CPB This book is intended for researchers designers and engineering technicians This book can also be a textbook for postgraduate students on mining engineering and other related subjects

Trends and Perspectives in Modern Computational Science George Maroulis, 2006-10-27 Contains a collection of the lectures of the invited speakers

presented at the International Conference of Computational methods in Science and Engineering ICCMSE 2006 held in Chania Greece October 2006 This book presents developments of Computational Science pertinent to Physics Chemistry Biology Medicine Mathematics and Engineering *Electronic and Photoelectron Spectroscopy* Andrew M. Ellis,Miklos Feher,Timothy G. Wright,2005-01-13 Electronic and photoelectron spectroscopy can provide extraordinarily detailed information on the properties of molecules and are in widespread use in the physical and chemical sciences Applications extend beyond spectroscopy into important areas such as chemical dynamics kinetics and atmospheric chemistry This book aims to provide the reader with a firm grounding of the basic principles and experimental techniques employed The extensive use of case studies effectively illustrates how spectra are assigned and how information can be extracted communicating the matter in a compelling and instructive manner Topics covered include laser induced fluorescence resonance enhanced multiphoton ionization cavity ringdown and ZEKE spectroscopy The volume is for advanced undergraduate and graduate students taking courses in spectroscopy and will also be useful to anyone encountering electronic and or photoelectron spectroscopy during their research *Job Matching, Wage Dispersion, and Unemployment* Dale T. Mortensen,Christopher A. Pissarides,2011-04-28 A selection of key papers from the winners of the Nobel Memorial Prize 2010 It features their most important work on unemployment labour market dynamics and the equilibrium search model *Research Paper PNW.* ,1978

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