

Compound	a_0 (Å)	c/a	B_0 (GPa)
GaN	3.215	1.639	186.52
	3.221 ^a	1.629 ^b	184.85 ^b
	3.190 ^c	-	188.00 ^d
MnN	4.271	-	291.50 ^e
	4.300 ^f		
	4.320 ^g		
1x1-MnN/GaN	3.198	1.626	198.10

^{a,b,e,f} Theoretical reference [11,12,15,16].

^{c,d,g} Experimental reference [13,14,17].

Equilibrium Structural Parameters

Terry C. Jones



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

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 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

Controlled Polymerization and Polymeric Structures Akihiro Abe, Kwang-Sup Lee, L. Leibler, Shiro Kobayashi, 2014-07-08 Advances in Polymer Science enjoys a longstanding tradition and good reputation in its community Each volume is dedicated to a current topic and each review critically surveys one aspect of that topic to place it within the context of the volume The volumes typically summarize the significant developments of the last 5 to 10 years and discuss them critically presenting selected examples explaining and illustrating the important principles and bringing together many important references of primary literature On that basis future research directions in the area can be discussed Advances in Polymer Science volumes thus are important references for every polymer scientist as well as for other scientists interested in polymer science as an introduction to a neighboring field or as a compilation of detailed information for the specialist **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 *Thixoforming* Gerhard Hirt, Reiner Kopp, 2009-02-11 Offering a sound technological overview while also including the fundamental aspects this book provides the knowledge needed to master the highly challenging process

characteristics for successful application in industrial production It summarizes the first hand experience gained from twelve years of collaborative research covering materials science rheology casting and forming control and surface technology as well as the modeling of flow behavior tool engineering and systems engineering and thus treats all the vital aspects of this field For materials scientists physicists engineers and those working in the metal processing industry Handbook of Industrial Organization ,2021-12-09 Handbook of Industrial Organization Volume Four highlights new advances in the field with this new volume presenting interesting chapters written by an international board of expert authors Presents authoritative surveys and reviews of advances in theory and econometrics Reviews recent research on capital raising methods and institutions Includes discussions on developing countries **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 **Neutron Scattering** Thomas Brückel,Gernot Heger,Dieter Richter,Georg Roth,Reiner Zorn,2014 Neutron Scattering ,2012

Handbook of Regional and Urban Economics ,2025-08-01 Regional and urban economics in the last ten years has benefited from the simultaneous development of new theoretical techniques new sources of geographic information systems GIS data rapid advances in computing power machine learning and artificial intelligence and renewed public policy interest in transportation infrastructure and appropriate policies towards places left behind by globalization and technological change This volume reviews this recent wave of research and highlights promising areas for further research Chapters include Quantitative Regional Economics Quantitative Urban Economics Optimal Spatial Policies Spatial Dynamics Transportation Housing Supply and Housing Affordability Spatial Sorting and Inequality Local Labor Markets Spatial Environmental Economics Spatial Economics for Low and Middle Income Countries and New Data and Insights for Regional and Urban Economics Comprehensive coverage of frontier research topics such as quantitative regional economics quantitative urban economics and spatial dynamics Contributions from some of the leading research scholars in regional and urban economics Advanced treatment of optimal spatial policies including place based policies and transport infrastructure investments

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

Structure Elucidation in Organic Chemistry Maria-Magdalena Cid, Jorge Bravo, 2014-12-17 Intended for advanced readers this is a review of all relevant techniques for structure analysis in one handy volume As such it provides the latest knowledge on spectroscopic and related techniques for chemical structure analysis such as NMR optical spectroscopy mass spectrometry and X ray crystallography including the scope and limitation of each method As a result readers not only become acquainted with the techniques but also the advantages of the synergy between them This enables them to choose the correct analytical method for each problem saving both time and resources Special emphasis is placed on NMR and its application to absolute configuration determination and the analysis of molecular interactions Adopting a practical point of view the author team from academia and industry guarantees both solid methodology and applications essential for structure determination equipping experts as well as newcomers with the tools to solve any structural problem

Single Molecule Tools, Part B: Super-Resolution, Particle Tracking, Multiparameter, and Force Based Methods, 2010-07-09 Single molecule tools have begun to revolutionize the molecular sciences from biophysics to chemistry to cell biology They hold the promise to be able to directly observe previously unseen molecular heterogeneities quantitatively dissect complex reaction kinetics ultimately miniaturize enzyme assays image components of spatially distributed samples probe the mechanical properties of single molecules in their native environment and just look at the thing as anticipated by the visionary Richard Feynman already half a century ago Single Molecule Tools Part B Super Resolution Particle Tracking Multiparameter and Force Based Methods captures a snapshot of this vibrant rapidly expanding field presenting articles from pioneers in the field intended to guide both the newcomer and the expert through the intricacies of getting single molecule tools Includes time tested core methods and new innovations applicable to any researcher employing single molecule tools Methods included are useful to both established researchers and newcomers to the field Relevant background and reference information given for procedures can be used as a guide to developing protocols in a number of disciplines

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

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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 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, 1962 **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

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 *Band Structure Engineering in Semiconductor Microstructures* R.A. Abram, M. Jaros, 2012-12-06 This volume contains the proceedings of the NATO Advanced Research Workshop on Band Structure Engineering in Semiconductor Microstructures held at Il Ciocco Castelveccchio Piacenza in Tuscany between 10th and 15th April 1988 Research on semiconductor microstructures has expanded rapidly in recent years as a result of developments in the semiconductor growth and device fabrication technologies The emergence of new semiconductor structures has facilitated a number of approaches to producing systems with certain features in their electronic structure which can lead to useful or interesting properties The interest in band structure engineering has stimulated a variety of physical investigations and novel device concepts and the field now exhibits a fascinating interplay between pure physics and device technology Devices based on microstructures are useful vehicles for fundamental studies but also new device ideas require a thorough understanding of the basic physics Around forty researchers gathered at Il Ciocco in the Spring of 1988 to discuss band structure engineering in semiconductor microstructures

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