

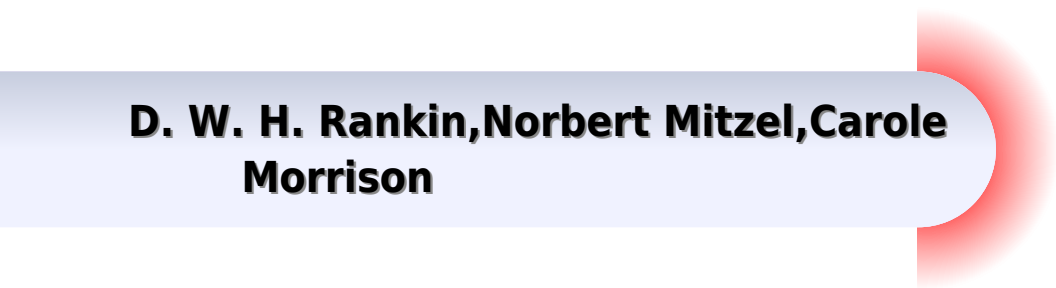
Stereochemical
Applications of Gas-Phase
Electron Diffraction - Part
B (Methods in
Stereochemical Analysis)

Hargittai, I

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Stereochemical Applications Of Gas Phase Electron Diffraction

D. W. H. Rankin, Norbert Mitzel, Carole Morrison



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Stereochemical Applications of Gas-Phase Electron Diffraction István Hargittai, M. Hargittai, 1988-10-01 This collection of twenty six articles by leading experts is the first truly comprehensive account of the gas phase electron diffraction technique It is written for the non specialist users of structural information Part A discusses the development and present capabilities of gas electron diffraction Several contributions deal with the combined application of various techniques Part B contains the structural information and also presents trends and interpretations of structural variations *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 Beitr ge stammen von Autoren aus neun L ndern aus allen f hrenden auf diesem Gebiet arbeitenden Forschungslaboratorien Das Buch enth lt einen einf hrenden Artikel von Herman Mark dem Pionier der Gasphasenelektronenbeugung und ein Vorwort von Jerome Karle dem Chemie Nobelpreistr ger von 1985 Es wird nur zusammen in zwei Teillb nden abgegeben Teil A beschreibt Entwicklung und derzeitige M glichkeiten der Methode darunter auch ihre Kombination mit anderen Verfahren Teil B enth lt Ergebnisse von Strukturbestimmungen f r zahlreiche Verbindungsklassen Er dient als umfassendes zuverl ssiges Nachschlagewerk und bringt gleichzeitig Trends und Interpretationen von Strukturvariationen Stereochemical Applications of Gas-phase Electron Diffraction: Structural

information for selected classes of compounds István Hargittai, Magdolna Hargittai, 1988 *Equilibrium Structure of Free Molecules* Natalja Vogt, Jean Demaison, 2023-12-06 The properties of chemical pharmaceutical and biological compounds depend mainly on their molecular structure whose determination is of fundamental interest This book examines and systematizes more than three hundred striking structural determinations of free molecules Featuring high quality structural

data and presenting modern techniques of their determinations by quantum chemistry high resolution spectroscopy and electron diffraction the book is an indispensable resource for graduate students and professional scientists specializing in structural chemistry and other related fields

Structure Data of Free Polyatomic Molecules Natalja Vogt, Jürgen Vogt, 2020-01-02 This handbook presents structural data on free polyatomic molecules Since the structure of molecules defines the chemical physical and biological properties of matter this information is crucial for understanding explaining and predicting chemical reactions and biochemical processes developing new drugs and materials as well as studying interstellar media Covering the structural data published between 2009 and 2017 this book supplements the previous Landolt B rnstein volumes Structure Data of Free Polyatomic Molecules eds K Kuchitsu N Vogt M Tanimoto which included data from the literature published up to 2008 It systematizes and describes peculiarities of molecular structures for about 1000 compounds studied mainly by gas phase electron diffraction and rotational spectroscopy All structures are given in three dimensional representations

Stereochemistry of Organic Compounds Ernest L. Eliel, Samuel H. Wilen, 1994-09-28 Stereochemistry of Organic Compounds The first fully referenced comprehensive book on this subject in more than thirty years Stereochemistry of Organic Compounds contains up to date coverage and insightful exposition of all important new concepts developments and tools in the rapidly advancing field of stereochemistry including Asymmetric and diastereoselective synthesis Conformational analysis Properties of enantiomers and racemates Separation and analysis of enantiomers and diastereoisomers Developments in spectroscopy including NMR chromatography and molecular mechanics as applied to stereochemistry Prostereoisomerism Conceptual foundations of stereochemistry including terminology and symmetry concepts Chiroptical properties Written by the leading authorities in the field the text includes more than 4 000 references 1 000 illustrations and a glossary of stereochemical terms

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

Advances in Molecular Structure Research , 1997-03-08 Advances in Molecular Structure Research

Molecular Orbital Calculations for Biological Systems Anne-Marie Sapse, 1998-11-12 Molecular Orbital Calculations for Biological Systems is a hands on guide to computational quantum chemistry and its applications in organic chemistry biochemistry and molecular biology With improvements in software molecular modeling

techniques are now becoming widely available they are increasingly used to complement experimental results saving significant amounts of lab time Common applications include pharmaceutical research and development for example ab initio and semi empirical methods are playing important roles in peptide investigations and in drug design The opening chapters provide an introduction for the non quantum chemist to the basic quantum chemistry methods ab initio semi empirical and density functionals as well as to one of the main families of computer programs the Gaussian series The second part then describes current research which applies quantum chemistry methods to such biological systems as amino acids peptides and anti cancer drugs Throughout the authors seek to encourage biochemists to discover aspects of their own research which might benefit from computational work They also show that the methods are accessible to researchers from a wide range of mathematical backgrounds Combining concise introductions with practical advice this volume will be an invaluable tool for research on biological systems

4D Electron Microscopy Ahmed H. Zewail, John Meurig Thomas, 2010 Structural phase transitions mechanical deformations and the embryonic stages of melting and crystallization are examples of phenomena that can now be imaged in unprecedented structural detail with high spatial resolution and ten orders of magnitude as fast as hitherto No monograph in existence attempts to cover the revolutionary dimensions that EM in its various modes of operation nowadays makes possible The authors of this book chart these developments and also compare the merits of coherent electron waves with those of synchrotron radiation They judge it prudent to recall some important basic procedural and theoretical aspects of imaging and diffraction so that the reader may better comprehend the significance of the new vistas and applications now afoot This book is not a vade mecum numerous other texts are available for the practitioner for that purpose

Combustion Efficiency and Air Quality Istvan Hargittai, T. Vidóczy, 2012-12-06 In this timely volume scientists examine the physical structural and analytical chemistry of fuel combustion Their contributions also address the issue of combustion efficiency and how air quality can be protected or improved Supported by numerous illustrations this volume be appreciated by researchers and students working in various areas of chemistry

Electron Crystallography Thomas E. Weirich, János L. Lábár, Xiaodong Zou, 2006-08-18 During the last decade we have been witness to several exciting achievements in electron crystallography This includes structural and charge density studies on organic molecules complicated inorganic and metallic materials in the amorphous nano meso and quasi crystalline state and also development of new software tailor made for the special needs of electron crystallography Moreover these developments have been accompanied by a now available new generation of computer controlled electron microscopes equipped with high coherent field emission sources cryo specimen holders ultra fast CCD cameras imaging plates energy filters and even correctors for electron optical distortions Thus a fast and semi automatic data acquisition from small sample areas similar to what we today know from imaging plates diffraction systems in X ray crystallography can be envisioned for the very near future This progress clearly shows that the contribution of electron crystallography is quite unique as it enables to reveal the intimate

structure of samples with high accuracy but on much smaller samples than have ever been investigated by X ray diffraction As a tribute to these tremendous recent achievements this NATO Advanced Study Institute was devoted to the novel approaches of electron crystallography for structure determination of nanosized materials **Time-resolved Diffraction** J. R Helliwell, P. M. Rentzepis, 1997-12-18 The acceleration of the technical capabilities of X ray electron and neutron diffraction techniques in recent years has been driven by developments in synchrotron and neutron sources detectors and computers These allow the rapid and repeated acquisition of diffraction data as a chemical and biological structural process proceeds following its initiation This opens up completely new studies from timescales ranging from the sub picosecond at the fastest through all the time domains up to kiloseconds for the slower molecular processes *Selected Topics on Electron Physics* D. Murray Campbell, Hans Kleinpoppen, 2012-12-06 In the spring of 1970 Peter Farago organised a three day conference on Polarised Electron Beams at Carberry Tower near Edinburgh Although the development of the gallium arsenide source which was to revolutionise the world of experimental polarised electron physics was still some years in the future the meeting provided an important forum for the exchange of ideas among theoreticians and experimentalists engaged in both high and low energy electron collision studies As soon as the decision had been taken to hold the 5th European Conference on Atomic and Molecular Physics in Edinburgh in 1995 it occurred to the editors of the present volume that it would be highly appropriate to mark the twenty fifth anniversary of the Carberry Tower Conference by organising an ECAMP satellite meeting in honour of Peter Farago The opportunity to pay tribute to Peter s many important contributions in the broad field of electron physics attracted colleagues from all over the world to the symposium which was held in the rooms of the Royal Society of Edinburgh on 31st March and 1st April 1995 Peter himself now Professor Emeritus at the University of Edinburgh was present throughout the meeting We were particularly happy to welcome back to Edinburgh many participants in the original Carberry Tower conference these included Professor P G Burke Professor J Kessler Professor E Reichert and Professor H C Siegmann whose review papers had been highlights of the 1970 meeting **Structural Methods in Molecular Inorganic Chemistry** D. W. H. Rankin, Norbert Mitzel, Carole Morrison, 2013-01-02 Determining the structure of molecules is a fundamental skill that all chemists must learn Structural Methods in Molecular Inorganic Chemistry is designed to help readers interpret experimental data understand the material published in modern journals of inorganic chemistry and make decisions about what techniques will be the most useful in solving particular structural problems Following a general introduction to the tools and concepts in structural chemistry the following topics are covered in detail computational chemistry nuclear magnetic resonance spectroscopy electron paramagnetic resonance spectroscopy Mossbauer spectroscopy rotational spectra and rotational structure vibrational spectroscopy electronic characterization techniques diffraction methods mass spectrometry The final chapter presents a series of case histories illustrating how chemists have applied a broad range of structural techniques to interpret and understand chemical systems Throughout the

textbook a strong connection is made between theoretical topics and the real world of practicing chemists Each chapter concludes with problems and discussion questions and a supporting website contains additional advanced material Structural Methods in Molecular Inorganic Chemistry is an extensive update and sequel to the successful textbook Structural Methods in Inorganic Chemistry by Ebsworth Rankin and Cradock It is essential reading for all advanced students of chemistry and a handy reference source for the professional chemist

In Our Own Image Istvan Hargittai, Magdolna Hargittai, 2012-12-06

The title of our volume refers to what is well described by the following two quotations God created man in his own image and Man creates God in his own image 2 Our approach to symmetry is subjective and the term personal symmetry reflects this approach in our discussion of selected scientific events We have chosen six icons to symbolize six areas Kepler for modeling Fuller for new molecules Pauling for helical structures Kitaigorodskii for packing Bernal for quasicrystals and Curie for dissymmetry For the past three decades we have been involved in learning thinking speaking and writing about symmetry This involvement has augmented our principal activities in molecular structure research Our interest in symmetry had started with a simple fascination and has evolved into a highly charged personal topic for us At the start of this volume we had had several authored and edited symmetry related books behind 3 us We owe a debt of gratitude to the numerous people whose interviews are quoted 4 in this volume We very much appreciate the kind and gracious cooperation of Edgar J Applewhite Washington DC Lawrence S Bartell University of Michigan R

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