

**Modelling of Structure
and Properties of
Molecules (Ellis Horwood
Series in Analytical
Chemistry)**

Maksic, Z.B.

Modelling Of Structure And Properties Of Molecules

Frank Northen Magill

Modelling Of Structure And Properties Of Molecules:

Modelling of Structure and Properties of Molecules Zvonimir B. Maksić, 1987 **Modelling of Structure and Properties of Molecules** Z.B. Maksic, 1987-06-01 *Molecular Simulation Studies on Thermophysical Properties* Gabriele Raabe, 2017-02-17 This book discusses the fundamentals of molecular simulation starting with the basics of statistical mechanics and providing introductions to Monte Carlo and molecular dynamics simulation techniques. It also offers an overview of force field models for molecular simulations and their parameterization with a discussion of specific aspects. The book then summarizes the available know how for analyzing molecular simulation outputs to derive information on thermophysical and structural properties. Both the force field modeling and the analysis of simulation outputs are illustrated by various examples. Simulation studies on recently introduced HFO compounds as working fluids for different technical applications demonstrate the value of molecular simulations in providing predictions for poorly understood compounds and gaining a molecular level understanding of their properties. This book will prove a valuable resource to researchers and students alike. **Molecular Simulation Methods for Predicting Polymer Properties** Vassiliios Galiatsatos, 2005-02-03 Among the thousands of synthesized polymers new polymeric substances and materials with new often unusual properties often arise. Consequently this presents a problem in determining the physical properties of polymers and thus makes it difficult to ascertain how to synthesize polymers with desired properties. This book discusses what molecular modelling can do to predict the properties of realistic polymer systems. Organized by property each chapter will address the methods one may use to study the particular system. Focuses on polymer properties rather than methods making it more accessible to the average scientist/engineer. All important polymers will be covered such as amorphous polymers, semicrystalline polymers, elastomers, emulsions, polymer interfaces and surfaces. Chapters contributed by experts in the field. Discusses current commercial software used in molecular simulation. **Molecular Modeling and Dynamics of Bioinorganic Systems** Lucia Banci, Peter Comba, 2012-12-06 A unique selection of papers on the most recent progress in the modelling of biological molecules containing metal ions. New approaches and techniques in this field are allowing researchers to discuss structures, electronic properties and reaction mechanisms of metalloproteins on the basis of computational studies. The book discusses different approaches in the development of new force fields and their application to the computation of the structures, electronic properties and dynamics of bioinorganic compounds as well as quantum mechanical and integrated QM/MM methods for understanding the function of metalloenzymes and the calculation of electrostatic interactions. **Structural and Electronic Properties of Molecular Nanostructures** Hans Kuzmany, 2002-10-04 The Winterschool provides a platform for reviewing and discussing new developments in the field of structural, electronic and mechanical properties of molecular nanostructures and their applications. Subjects included are carbon nanotubes, mechanical and electrical properties, carbon nanotubes structure and functionalization, fullerenes and fullerene derivatives, molecular clusters, polymeric carbon phases.

single molecule experiments chemistry of molecular nanostructures application of molecular nanostructures layer by layer systems and hybrid materials biological nanostructures and molecular machines Computer Generated Physical Properties Stan Bumble,1999-06-01 Computer Generated Physical Properties offers the environmental scientist a basis to predict the properties of molecules and reengineer them to remove those properties that are harmful to the environment This technology is currently used in other fields and is now becoming popular in the environmental engineering field because of its pollution prevention and waste reduction capabilities This book interdisciplinary in scope treats the physical properties of matter as generated by computers It covers a wide variety of topics pointing towards synthesizing new molecules to substitute for reactants intermediaries and products in industrial processes with better physical and environmental properties than the original The author achieves this with a spreadsheet program called SYNPROPS that operates on a PC computer with optimization features A radar type graph one for each property visually sorts the various groups in order of their contribution to the property creating the necessity for a computer to obtain answers for the structure of the optimum molecules for substitution or synthesis The author discusses applications to biologically active molecules without side effects including antineoplastic drugs Additionally he demonstrates model compounds and the applications of SYNPROPS optimization and substitution This book has everything you need to know about deriving properties and combinational chemistry from molecular structure

Physical Properties and Thermodynamic Behaviour of Minerals Ekhard K.H. Salje,1988-01-31

The role played by earth sciences in the scientific community has changed considerably during this century Since the revolutionary discoveries of global processes such as plate tectonics there has been an increasing awareness of just how fundamental many of the mechanisms which dominate in these processes depend on the physical properties of the materials of which the earth is made One of the prime objectives of mineral sciences is now to understand and predict these properties in a truly quantitative manner The macroscopic properties which are of most immediate interest in this context fall within the conventional definitions of thermodynamics magnetism elasticity dielectric susceptibilities conductivity etc These properties reflect the microscopic contributions at an atomistic level of harmonic and anharmonic lattice vibrations ionic and electronic transport as well as a great variety of ordering and clustering phenomena The advances made by solid state physicists and chemists in defining the underlying phenomena involved in the thermal evolution of materials have stimulated major new research initiatives within the Earth Sciences Earth Scientists have combined to form active groups within the wider community of solid state and materials scientists working towards a better understanding of those physical processes which govern not only the behaviour of simple model compounds but also that of complex materials like minerals Concomitant with this change in direction has come an increasing awareness of the need to use the typical working tools of other disciplines

Acta Crystallographica ,1925 Science John Michels (Journalist),1924 Transactions of the Faraday Society Faraday Society,1923 **The Molecular Basis of Membrane Function** Society of General Physiologists,1969 Includes

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