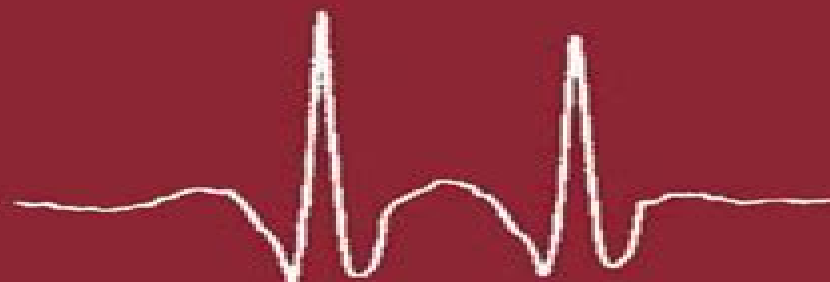

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SPECTROSCOPIC AND
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Spectroscopic And Computational Studies Of Supramolecular Systems

John A. Ripmeester, Saman Alavi



Spectroscopic And Computational Studies Of Supramolecular Systems:

Spectroscopic and Computational Studies of Supramolecular Systems J.E. Davies, 2013-04-17 Physical techniques such as X ray crystallography IR spectroscopy and solution phase NMR spectroscopy have played key roles in the development of supramolecular chemistry In recent years other spectroscopic techniques have been applied expanding the range of information obtainable The most widely used technique is solid state NMR spectroscopy but techniques such as neutron scattering and NQR spectroscopy can yield significant information Computational approaches are now becoming powerful complementary methods to experimental techniques and this book reviews the application of these methods to supramolecular systems The ten chapters provide up to date information on the applications of spectroscopic and computational techniques to a wide range of supramolecular systems Solid State NMR Studies of Host Guest Materials Infrared Studies of Zeolite Complexes NQR Studies of Inclusion Compounds Neutron Scattering Studies of Zeolite Complexes Solid State NMR Studies of Catalytic Reactions on Molecular Sieves Recent Advances in Computational Studies of Zeolites Theoretical Studies of Cyclodextrins and their Inclusion Complexes Computer Modelling of the Structures of Host Guest Complexes Computational Studies of Clathrate Hydrates Ab initio Electronic Structure Calculations on Endohedral Complexes of the C60 Cluster This timely book will prove to be of great value to supramolecular researchers who are familiar with the spectroscopic techniques but who wish to extend their knowledge of the computational methods and vice versa to supramolecular researchers working in allied areas whose work would benefit from applying spectroscopic and computational methods and finally to workers just entering the fascinating area of supramolecular chemistry

Spectroscopic and Computational Studies of Supramolecular Systems J. E. Davies, 2014-01-15 Host-Guest Chemistry Brian D. Wagner, 2020-10-26 This textbook addresses the chemical and physicochemical principles of supramolecular host guest chemistry in solution It covers the thermodynamics and dynamics of inclusion and highlights several types of organic hosts Various applications of host guest chemistry in analytical and environmental chemistry as well as pharmaceutical and chemical industry demonstrate the versatile usability of molecular cages Clathrate Hydrates, 2 Volumes John A. Ripmeester, Saman Alavi, 2022-05-31 Clathrate Hydrates All inclusive reference on clathrate hydrates from a molecular perspective Clathrate hydrates are crystalline water based inclusion compounds many of which form at high pressures and low temperatures Molecular science has provided the foundation for many areas of modern hydrate research and applications ranging from desalination processes to flow assurance in oil and gas pipelines Clathrate Hydrates provides detailed information on the molecular science aspects of hydrate research covering the structural compositional spectroscopic thermodynamic and mechanical properties of clathrate hydrates as well as simulation methods and selected engineering applications Edited and authored by recognized leaders in the field this comprehensive resource introduces readers to clathrate hydrates and reviews the state of the art of the field In depth chapters address different areas of

specialization such as characterization of clathrate hydrates using NMR spectroscopy infrared and Raman spectroscopy and X ray and neutron diffraction and scattering Highlights recent developments in clathrate hydrate research and applications such as natural gas recovery desalination and gas separation Reviews various molecular simulation methods for characterizing clathrate hydrates including quantum mechanical calculations and Monte Carlo results Contains tables of known guest molecules summaries of structural and physical properties and different classes of clathrate hydrate phase equilibria Introduces unconventional guest host interactions related non hydrate clathrates and space filling cages using the Frank Kasper approach Covers the molecular motion of guest and host molecules and the relationship between cage geometry and guest dynamics Presents the rate and mechanisms of hydrate formation and decomposition from both macroscopic and microscopic points Clathrate Hydrates Molecular Science and Characterization is an indispensable reference for materials scientists physical chemists chemical engineers geochemists and graduate students in relevant areas of science and engineering Handbook of Zeolite Science and Technology Scott M. Auerbach, Kathleen A. Carrado, Prabir K. Dutta, 2003-07-31 The Handbook of Zeolite Science and Technology offers effective analyses of salient cases selected expressly for their relevance to current and prospective research Presenting the principal theoretical and experimental underpinnings of zeolites this international effort is at once complete and forward looking combining fundamental

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Years of Condensed Matter and Related Physics Raymond L. Orbach Symposium 1995, University of California, Riverside, Daniel W. Hone, 1996 The 9 papers of this volume were presented at the March 1995 Symposium honoring Raymond L Orbach on his 60th birthday The range of topics reflects the breadth of Dr Orbach's own research It includes magnetism and transport in nanostructures crystal fields in superconducting cuprates fractons and scaling in disordered systems glassy relaxation inelastic atom crystal scattering bosonization in d 1 and microwave effects in superconductors

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