



Supramolecular Chemistry

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Computational Approaches In Supramolecular Chemistry Nato Science Series C

Lingsheng Yao



Computational Approaches In Supramolecular Chemistry Nato Science Series C:

Computational Approaches in Supramolecular Chemistry G. Wipff, 2012-12-06 Supramolecular chemistry has been defined by J M Lehn as a highly interdisciplinary field of science covering the chemical physical and biological features of chemical species of higher complexity that are held together and organized by means of intermolecular noncovalent binding interactions Science 1993 Recognition reactivity and transport represent three basic functional features in essence dynamics which may be translated into structural features The purpose of the NATO workshop which took place September 15 1993 at the Bischensberg near Strasbourg was to present computations which may contribute to the atomic level understanding of the structural and thermodynamical features involved in the processes of molecular recognition and supramolecular organization of supramolecular modeling Other The main focus was therefore on the many facets applications of computers in chemistry such as automation simulation of processes procedures for fitting kinetic or thermodynamic data computer assisted synthetic strategies use of data bases for structure elucidation or for bibliographic searches have an obvious impact in supramolecular chemistry as well but were not presented at the workshop

Supramolecular Science Rocco Ungaro, Enrico Dalcanale, 2012-12-06 A summary of all the most important aspects of supramolecular science from molecular recognition in chemical and biological systems to supramolecular devices materials and catalysis The 17 chapters cover calixarenes catenanes cavitands cholephanes dendrimers membranes and self assembly systems molecular modelling molecular level devices organic materials peptides and protein surfaces recognition of carbohydrates rotaxanes supramolecular catalysis A forward looking chapter written by J M Lehn indicated the future prospects for the entire field Audience Ph D students and young researchers in chemistry physics and biology

Advances in Microfluidic Technologies for Energy and Environmental Applications Yong Ren, 2020-05-20 Microfluidics have aroused a new surge of interest in recent years in environmental and energy areas and inspired novel applications to tackle the worldwide challenges for sustainable development This book aims to present readers with a valuable compendium of significant advances in applying the multidisciplinary microfluidic technologies to address energy and environmental problems in a plethora of areas such as environmental monitoring and detection new nanofluid application in traditional mechanical manufacturing processes development of novel biosensors and thermal management This book will provide a new perspective to the understanding of the ever growing importance of microfluidics

A Practical Guide to Supramolecular Chemistry Peter J. Cragg, 2005-11-04 A Practical Guide to Supramolecular Chemistry is an introductory manual of practical experiments for chemists with little or no prior experience of supramolecular chemistry Syntheses are clearly presented to facilitate the preparation of acyclic and macrocyclic compounds frequently encountered in supramolecular chemistry using straightforward experimental procedures Many of the compounds can be used to illustrate classic supramolecular phenomena for which clear directions are given or may be developed further as part of the reader's own research The book also describes techniques commonly used in the analysis of

Introduction

Supramolecular Chemistry Helena Dodziuk, 2007-05-08 A new rapidly progressing field on the crossroads among chemistry biochemistry physics and technology supramolecular chemistry has just emerged You have to be involved to know what s going on in this domain and to take part in the development This book will show you in a condensed form exciting phenomena unthinkable within the realm of classical organic chemistry for example alkali metal anions or cyclobutadiene stable for month at room temperature that not only provide the basis for revolutionizing numerous branches of industry but also improve our understanding of the functioning of living organisms and of the origin of life Designing supramolecular systems with desired properties will among others make chemical industry cleaner and more safe electronics smaller by developing devices composed of single molecule or molecular aggregate It will also entirely change the way we use energy resources In addition it will also transform the pharmaceutical industry and medicine by developing new ways of drugs administration and new composite biocompatible materials which will serve as implants of new generation changing dentistry surgery and other branches of medicine You cannot afford to stand apart With its brief but comprehensive and vivid presentation including the latest development Introduction to Supramolecular Chemistry is the best method to get into this domain This book provides an excellent summary of information scattered across the literature The brief but comprehensive coverage of the whole field including practically all important group of compounds forming aggregates in particular crown ethers cavitands fullerenes cyclodextrins and their complexes provisioning full references for the discussed subjects make this book of value not only for Ph D students and non specialists in this domain but also for those working in the field The book has been found to be a particularly useful resource for students and more generally for those wanting to get the up to date concise account of this exciting field □□□□□□□□□□□□□□□□□□□□ , 1997 Kokuritsu Kokkai Toshokan shozō kagaku qijutsu kankei Ōbun kaigiroku mokuroku Kokuritsu Kokkai Toshokan (Japan), 1997 Biological Membranes Kenneth M.

Merz, Benoit Roux, 2012-12-06 The interface between a living cell and the surrounding world plays a critical role in numerous complex biological processes. Sperm egg fusion, virus cell fusion, exocytosis, endocytosis, and ion permeation are a few examples of processes involving membranes. In recent years, powerful tools such as X-ray crystallography, electron microscopy, nuclear magnetic resonance, and infra-red and Raman spectroscopy have been developed to characterize the structure and dynamics of biomembranes. Despite this progress, many of the factors responsible for the function of

biomembranes are still not well understood The membrane is a very complicated supramolecular liquid crystalline structure that is largely composed of lipids forming a bilayer to which proteins and other biomolecules are anchored Often the lipid bilayer environment is pictured as a hydrophobic structureless slab providing a thermodynamic driving force to partition the amino acids of a membrane protein according to their solubility However much of the molecular complexity of the phospholipid bilayer environment is ignored in such a simplified view It is likely that the atomic details of the polar head group region and the transition from the bulk water to the hydrophobic core of the membrane are important An understanding of the factors responsible for the function of biomembranes thus requires a better characterization at the molecular level of how proteins interact with lipid molecules of how lipids affect protein structure and of how lipid molecules might regulate protein function

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