

QUANTUM THEORY OF POLYMERS AS SOLIDS

János J. Ladik

Quantum Theory Of Polymers As Solids

Anthony S. Fauci



Quantum Theory Of Polymers As Solids:

Quantum Theory of Polymers as Solids Janos J. Ladik, 2012-12-06 The goal of this monograph is to summarize the different quantum mechanical methods developed in the last 20 years to treat the electronic structure of polymers. Owing to the nature of the problem these methods consist of a mixture of quantum chemical and solid state physical techniques. The theory described in Part I treats besides the Hartree Fock problem the electron correlation and it has also been developed for disordered polymeric systems. Though for obvious reasons the book could not include all the existing calculations each new method described is illustrated by a few applications with a discussion of the numerical results obtained. Far more details see the Introduction to Part I. The second part contains the theoretical calculation of different properties of polymers based on the methods systematically introduced in the first part. The properties calculated include the electronic and vibrational spectra of polymers and the computation of their transport magnetic and mechanical properties. In cases where reliable experimental data are available the theoretical results are compared with them. Quantum Theory of Polymers as Solids

Janos J. Ladik, 1988 Solid State NMR of Polymers T. Asakura, Isao Ando, 1998-08-03 In polymer science and technology the advanced development of various new polymer materials with excellent properties and functions is desirable. For this purpose it is necessary to determine the exact relationship between physical properties and molecular structure dynamics with powerful techniques. One such technique is solid state NMR. Recently high resolution NMR studies of solids have been realized by using advanced pulse and mechanical techniques which has resulted in a variety of structural and dynamical information on polymer systems. Solid state NMR has provided characteristic information which cannot be obtained by other spectroscopic methods. This book is divided into two parts. The first part covers the principles of NMR important NMR parameters such as chemical shifts, relaxation times, dipolar interactions, quadrupolar interactions, pulse techniques and new NMR methods. In the second part applications of NMR to a variety of polymer systems in the solid state are described. Features of this book: Contains an up to date and comprehensive account of solid state NMR of polymers by leading researchers in the field. Provides a compilation of solid state NMR of polymers which makes it an ideal reference book for both NMR researchers and general polymer scientists. This book will be of interest to the NMR community and will be invaluable for both the beginner and the expert. *Quantum Chemistry of Polymers — Solid State Aspects* J. Ladik, J.

André, M. Seel, 2012-12-06 The NATO Advanced Study Institute on Quantum Chemistry of Polymers Solid State Aspects III as held at the MARITIM Congress Hotel Braunlage Harz in the Federal Republic of Germany from July 25 August 5 1983. We wish to express our deep gratitude to the NATO Scientific Affairs Division the main sponsor of the Institute and to the National Foundation for Cancer Research Bethesda Maryland for their substantial support. We sincerely thank Dr Craig Sinclair Director of the NATO Advanced Study Institutes program as well as the whole Advanced Study Institute Advanced Research Workshop Advisory Board of the NATO Scientific Affairs Division who have honored us by holding their external

annual meeting during this School in Braunlage We are very much indebted also to Dr Mario Di Lullo Director of the Advanced Research Workshop program of the NATO Scientific Affairs Division IIIho together IIIith Dr Sinclair has given a very informative lecture about the NATO ASI ARW programs Special thanks are due to Mr Franklin Salisbury Executive Director of the National Foundation for Cancer Research to Mrs Tamara Salisbury Deputy Director of the National Foundation for Cancer Research and to Dr Mary Hennen Aldridge President of the National Foundation for Cancer Research IIIho also honored the School IIIith their presence

Solid State NMR Spectroscopy for Biopolymers Hazime Saitô, Isao Ando, Akira Naito, 2006-08-05 Biopolymers are polymeric materials of biological origin including globular membrane and fibrous proteins polypeptides nucleic acids polysaccharides lipids etc and their assembly although preference to respective subjects may be different among readers who are more interested in their biological significance or industrial and or medical applications Nevertheless characterizing or revealing their secondary structure and dynamics may be an equally very important and useful issue for both kinds of readers Special interest in revealing the 3D structure of globular proteins nucleic acids and peptides was aroused in relation to the currently active Structural Biology X ray crystallography and multidimensional solution NMR spectroscopy have proved to be the standard and indispensable means for this purpose There remain however several limitations to this end if one intends to expand its scope further This is because these approaches are not always straightforward to characterize fibrous or membrane proteins owing to extreme difficulty in crystallization in the former and insufficient spectral resolution due to sparing solubility or increased effective molecular mass in the presence of surrounding lipid bilayers in the latter

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