
Description:
The progress in nuclear magnetic resonance (NMR) spectroscopy that took place during the last several decades is observed in both experimental capabilities and theoretical approaches to study the spectral parameters. The scope of NMR spectroscopy for studying a large series of molecular problems has notably broadened. However, at the same time, it requires specialists to fully use its potentialities. This is a notorious problem and it is reflected in the current literature where this spectroscopy is typically only used in a routine way. Also, it is seldom used in several disciplines in which it could be a powerful tool to study many problems. The main aim of this book is to try to help reverse these trends.

This book is divided in three parts dealing with 1) high-resolution NMR parameters; 2) methods for understanding high-resolution NMR parameters; and 3) some experimental aspects of high-resolution NMR parameters for studying molecular structures. Each part is divided into chapters written by different specialists who use different methodologies in their work. In turn, each chapter is divided into sections. Some features of the different sections are highlighted: it is expected that part of the readership will be interested only in the basic aspects of some chapters, while other readers will be interested in deepening their understanding of the subject dealt with in them.

- Shows how NMR parameters are useful for structure assignment as well as to obtain insight on electronic structures
- Emphasis on conceptual aspects

Contributions by specialists who use the discussed methodologies in their everyday work

Contents:
1. High Resolution Nuclear Magnetic Resonance Parameters for Understanding Molecules and their Electronic Structure, by Rubén Horacio Contreras
2. Brief account of non-relativistic theory of NMR parameters, Marta B. Ferraro and Rubén Horacio Contreras
3. Chemical shift in paramagnetic systems, by Juha Vaara
4. Relativistic effects on NMR parameters, by Jochen Autschbach
5. The polarization propagator approach as a tool to study electronic molecular structures from high resolution NMR parameters, by Gustavo A. Aucar
6. Analysis of contributions to spin-spin coupling constants by the natural J coupling method, by Jose Manuel García de la Vega
7. Electronic current densities induced by magnetic fields and nuclear magnetic dipoles. Theory and computation of NMR parameters, by Paolo Lazeretti
8. From NMR Spectra to Structure, by Julio C. Facelli
9. Transmission mechanisms of the Fermi-Contact term of spin-spin couplings, by Rubén Horacio Contreras
11. Chemical shift trends in light atoms, by Rubén Horacio Contreras

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