

Editorial

Special Issue on Recent Advances in Nuclear Magnetic Shielding Theory

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Received: 5 June 2002 / Published: 31 August 2002

Nuclear Magnetic Resonance Spectroscopy (NMR) is one of the most important tools to elucidate structure and environment. The NMR chemical shifts provide information on the geometry, conformation and electronic structure of molecules, polymers clusters and crystals.

During the last ten years the development of modern spectrometers, new experimental techniques, computers, supercomputers and the possibility of parallel processing, produced a formidable progress in combined experimental/theoretical approaches to describe NMR chemical shifts. The dependence of the chemical shifts on the molecular electronics and geometrical structure is established by quantum mechanical equations derived from first principles. Quantum-mechanical-chemical calculations produce three principal values of the chemical shift tensor. These principal values have more detailed information about structure of molecules and solids, as compared with isotropic chemical shifts. They permit deep insight into the structure of those molecules and solids.

The ability to relate the chemical shifts to structure using quantum mechanical methods opens up new possibilities for predicting and refining structures.

This issue is developed to “Recent advances in Nuclear Magnetic Shielding Theory”. The papers included in this volume provide an insight of the current state of the art in the calculation of the NMR chemical shielding.

The paper by Anderson *et al* employs a model to represent intermolecular effects and reproduce measured chemical shifts on a series of nitro- and amino-substituted nitrogen containing heterocycles that are of interest as potential non-sensitive explosives.

The contribution by E. Moore reviews recent *ab initio* calculations of cobalt NMR shielding and explores the variation of shielding with changes in the geometry of model complexes.

The paper of T. Alam reports the behavior of the chemical shielding anisotropy of ^{31}P in cyclic and acyclic phosphate clusters.

Ando *et al* contribute with an extensive study of proton chemical shifts behavior in a supermolecule of biological interest.

The paper from Romero and Aucar is a novel formalism to include self-energy corrections in NMR parameters within the Quantum Electrodynamics.