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Editorial

Special Issue on Nuclear Magnetic Resonance Spin–Spin Coupling Constants — Calculations and Measurements

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The importance of nuclear magnetic resonance (NMR) spectroscopy for the determination of three dimensional structures of even biomolecules has again been emphasized by last years Nobel prize. The strong geometry dependence of the indirect nuclear spin-spin coupling constants, *e.g.* the Karplus relationships for vicinal coupling constants, plays an important role in that context.

Recent years have not only seen the development of ever stronger magnets and thus higher resolution in NMR spectra but also a dramatic improvement in the accuracy of calculated spin-spin coupling constants. Several quantum mechanical methods for highly accurate calculations on model systems are nowadays available. Many research groups concentrate therefore on finer details such as relativistic effects and the effects of surrounding solvents and nuclear motion. Theoretical studies of indirect nuclear spin-spin coupling constants in larger molecules are also possible since the implementation of efficient and often accurate density functional theory methods.

This special issue contains a mixture of review and original articles, experimental and theoretical studies, studies of inter- and intramolecular spin-spin couplings, density functional theory and highly accurate *ab initio* calculations, application of established methods and presentation of new approaches, studies of geometry, solvent and electric field effects, in short a good representation of the diversity of different research activities within this field.

The contribution by I. Alkorta and J. Elguero reviews recent density functional theory and *ab initio* calculations of indirect nuclear spin-spin coupling constants through hydrogen-bonds and in van der Waals complexes.

Zaccari *et al.* contribute with a density functional theory study of solvent effects on indirect nuclear spin-spin coupling constants in acetaldehyde. They employed the polarizable continuum model but studied also specific solvent interactions with dimethylsulfoxide.

S. V. Zubkov and V. A. Chertkov show in their contribution how a continuous potential for the pseudorotation of disubstituted cyclopentanes can be derived from the complete analysis of the ^{1}H-NMR spectra of the respective compounds.

Ruud *et al.* present a new implementation of the polarizable continuum model for the calculation of solvent effects on indirect nuclear spin-spin coupling constants at the density functional theory and Hartree-Fock theory level. They illustrate their new approach by a study of the solvent effects on the indirect nuclear spin-spin coupling constants in benzene.

K. Jackowski reviews recent measurements of indirect nuclear spin-spin coupling constants and discusses the problem of density dependence and the effect of nuclear motion.

In the paper by M. Pecul and T. Helgaker the performance of density functional theory calculations of the indirect nuclear spin-spin coupling constants in ethane, methylamine and methanol is benchmarked against multiconfigurational self-consistent field and coupled-cluster singles-and-doubles calculations.

A. Wu and D. Cremer present density functional theory calculations of Karplus relationships for all indirect nuclear spin-spin coupling constants of the pseudorotating tetrahydrofuran.

The contribution by Bagno *et al.* is a density functional theory and *ab initio* study of through-space indirect nuclear spin-spin coupling constants in van der Waals dimers involving acetylene and in the structurally related covalent compound 4-ethynylphenanthrene.

Giribet *et al.* discuss electron correlation effects in *ab initio* calculations of intra- and intermolecular indirect nuclear spin-spin coupling constants in model systems with C-H…O interactions.

The paper by M. Grayson reports *ab initio* calculations of electric field derivatives of the geminal hydrogen-hydrogen indirect nuclear spin-spin coupling constants in methane and monosubstituted methane.

Finally, substituent effects on the indirect nuclear spin-spin coupling constants in imines and oximes are investigated by means of *ab initio* calculations in the contribution by Provasi *et al.*