Aims & scope

*MR* is devoted to the rapid publication of papers which are concerned with the development of magnetic resonance techniques, or in which the application of such techniques plays a pivotal part. Contributions from scientists working in all areas of NMR, ESR and NQR are invited, and papers describing applications in all branches of chemistry, structural biology and materials chemistry are published.

The journal is of particular interest not only to scientists working in academic research, but also those working in commercial organisations who need to keep up-to-date with the latest practical applications of magnetic resonance techniques.

Research articles

Aggregate formation of cyclopropyllithium leads in the presence of LiBr (1:1) in DEE to a mixed dimer and a static tetramer. In DEE/THF or THF, the mixed dimer is accompanied by a fluxional mixed tetramer. Dynamic NMR shows that both clusters are in equilibrium and that line-shape analysis yielded thermodynamic and kinetic parameters. Entropy data show that in the transition state of the tetramer–dimer equilibrium, the mixed dimers are still weakly coordinated.

NMR spectroscopy of organolithium compounds, part XXXIV: Cyclopropyllithium and lithium bromide (1:1) in diethylether/tetrahydrofuran—Identification of a fluxional mixed tetramer 131–138

O. Eppers and H. Günther

CASE-3D determination of relative configuration in polyhydroxilated compounds.  

Equation chapter 1 section 1 When not to rely on Boltzmann populations. Automated CASE-3D structure elucidation of hyacinthacines through chemical shift differences 139–144

A. Navarro-Vázquez
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Exponential dependencies between locally calculated geometric and magnetic indexes of aromaticity, harmonic oscillator model of aromaticity and nucleus independent chemical shifts (NICS)(0), NICS(1) and NICS(1)zz, and the number of conjugated benzene rings in linear acenes, from benzene to decacene were observed at B3LYP/6-311+G** level of theory.

Local aromaticity in polyacenes manifested by individual proton and carbon shieldings: DFT mapping of aromaticity 145–153
M. Gajda, Ł. Gajda, T. Kupka and T. Kar

Strong intramolecular hydrogen bonds and steric effects involving C=–S groups: An NMR and computational study 154–162
R. S. Elias, B. A. Saeed, F. S. Kamounah, F. Duus and P. E. Hansen

5-Acyl rhodanines and thiorhodanines with bulky substituents like tert-butyl and adamantoyl groups at the exocyclic double bond are very well suited to investigate the correlation between heavy atom X–X distances and hydrogen bond strength in conjunction with NMR. They are shown to exist in the intramolecular hydrogen-bonded enolic form. According to their OH chemical shifts and isotope effect on C13 chemical shifts as well as atoms in molecule calculations, the sterically hindered molecules with bulky substituents have stronger hydrogen bonds than those without steric compression.

Experimental estimates of compression heating and decompression cooling in ethylene glycol 163–169
J. Steele, J. Ames and M. Augustine

The well known temperature dependent 'H chemical shift difference Δσ between the hydroxyl and methylene protons in ethylene glycol is shown to also be pressure dependent. A Δσ surface as a function of temperature and pressure is constructed and used to experimentally determine the temperature rise during sample compression and recovery as equilibrium is established at elevated pressure. This work suggests that temperature changes during sample compression and decompression are not significant enough to interfere with protein folding studies.
The hidden sodium content in processed foods is an important factor that compromises the assessment of a healthy diet. The NMR-based method for sodium quantitation described in this work shows high precision and accuracy. This is a novel alternative for sodium quantitation using an efficient NMR-based methodology.

NMR spectral analysis of strongly second-order 6-, 8-, 9- and 10- spin-systems (1H-19F, 19F-19F, and 13C-19F) in perfluorotoluly- and tetrafluoro-pyridyl-aromatics using the lineshape method ANATOLIA. Mark Edgar*, Dee Hayward, Fatemeh Zeinali, Shahzad Riaz and George W. Weaver. A simple to use nuclear magnetic resonance analysis method (ANATOLIA) has been tested on complex 1H, 19F, and 13C multiplets. Up to 10 coupling nuclei were analysed in only 6 min using a laptop computer, and ANATOLIA was robust enough to be able to have excellent results from inaccurate input values. A fluorine fluorine coupling constant was attributed to a through-space interaction and modelled using Gaussian 09.

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Letter - spectral assignments

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1H, 13C and 15N NMR of spiro acridines integrated with pyrrole scaffolds
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