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Solution and solid-state NMR of paramagnetic molecules Paramagnetism is a unique tool in chemistry for the investigation of materials and complex systems including supramolecular assemblies, especially in the presence of internal flexibility.

Part of the field of competence of NMR is represented by

molecules with unpaired electrons, which are called paramagnetic. The presence of unpaired electrons is at the same time a drawback (negative effect) and a precious source of information about structure and dynamics.

Paramagnetic Effects in NMR

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Paramagnetic Effects in NMR - Outline and Useful References • Relaxation by electron spins - distance mapping • Field induced orientation - RDC measurements • Pseudo-contact shifts - distance and angle data • "Solution NMR of Paramagnetic

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 Paramagnetic Relaxation. Structural carbon atoms are black. The crevice in the molecule leaves room for a single water molecule (blue and green) to interact directly with the Gd +3 ion (inner sphere relaxation). Beyond this a second shell of other water molecules experience outer sphere relaxation.

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In a paramagnetic molecule, especially if it is not too large (large means long τ_r), τ_s usually dominates τ_c " τ_r ranges from 10-9 s (small protein) to 10-7 s (large for NMR) τ_s ranges from 10-13 s to 10-8 s; but values 10-13 to 10-10 most feasible for high-resolution NMR. Thus $\tau_{r-1} \ll \tau_{s-1}$ and τ_s dominates τ_c for metallo-proteins.

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Paramagnetic nuclear magnetic resonance spectroscopy

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NMR of Paramagnetic Molecules. International experts report the latest developments in NMR methodology as applied to strongly relaxed and shifted resonances, detail the theoretical aspects of paramagnetic shift and relaxation, and discuss the interpretive bases of these molecular properties in relation to the structure and function of various paramagnetic molecules.

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Paramagnetic nuclear magnetic resonance spectroscopy

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NMR spectroscopy at natural abundance. the NMR spectra of paramagnetic x-complexes. This has allowed the resolution of the signal splitting of Cp deuterons of 1 and 5 which could not be observed earlier in the ¹H NMR spectra. and large (2-4) signal splittings is discussed and related to an extended Huckel calculation.

NMR spectroscopy of paramagnetic complexes. Part 39 ...

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Paramagnetic relaxation - Questions and Answers in MRI

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