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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

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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 metalloproteins.

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In these molecules the electrons are paired together and their NMR spectra are straightforward to analyse since the signals are usually sharp and in distinctive regions according to the structure of the molecule. However, with NMR methods it is difficult to investigate the structure of paramagnetic compounds, which have unpaired

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electrons.

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**NMR techniques for
the analysis of
paramagnetic
materials ...**

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Description : NMR is a growing technique which represents a generalized, spread, common tool for spectroscopy and for structural and dynamic investigation. Part of the field of competence of NMR is represented by molecules with unpaired electrons, which are called paramagnetic.

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magnetic resonance
spectroscopy refers to
nuclear magnetic
resonance (NMR)
spectroscopy of
paramagnetic
compounds. [1] [2]
Although most NMR

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measurements are conducted on diamagnetic compounds, paramagnetic samples are also amenable to analysis and give rise to special effects indicated by a wide chemical shift range and broadened signals.

Paramagnetic nuclear magnetic resonance spectroscopy ...

Paramagnetic NMR I.

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Overview of

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of Paramagnetic Shifts

Scalar / Contact Dipolar
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This division is really
an artifact of viewing
molecules through

LCAO-MOT: Both Shifts
are due to the same
coupling phenomenon
of electron mag
moment coupling to
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7

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Paramagnetic NMR

NMR is a growing technique which represents a generalized, spread, common tool for spectroscopy and for structural and dynamic investigation. Part of the field of competence of NMR is represented by molecules with unpaired electrons, which are called paramagnetic.

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solution NMR to refine structures (22), to investigate protein-protein interactions (23, 24), or to monitor dynamics (25, 26). Small paramagnetic molecules have been studied through magic angle spinning (MAS) SSNMR for de-cades (27-33).

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Guidelines are provided to predict the order of magnitude of relaxation rates. It is

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shown that DFT-predicted paramagnetic shifts can greatly assist in obtaining and understanding the NMR spectra of paramagnetic molecules, which generally require different experimental strategies and exhibit problems in detection and assignment.

Predicting the NMR Spectra of

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Chemistry Elsevier,
Amsterdam, 2001. The
book presents the
basic theory of the
unpaired electron-
nucleus coupling and
the consequences on
nuclear chemical shift
and relaxation.

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Solution NMR of Paramagnetic Molecules

The characterization of active catalyst systems based on routine techniques has its limitations due to the fact that the complexes of the 3d metals are frequently paramagnetic compounds. 18 However, recent studies have shown that particularly

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paramagnetic NMR can serve as a powerful tool for the in situ identification as well as characterization of 3d metal complexes. 19 While the theoretical ...

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