

European Network on NMR Relaxometry

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Relaxation measurements using Nuclear Quadrupole Resonance Spectroscopy on Bi-aryl compounds

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Motivation and Introduction

Nuclear Quadrupole Resonance (NQR) properties are of major interest in exploiting a relaxation enhancing effect referred to as *Quadrupolar Relaxation Enhancement* (QRE)¹. In an external magnetic field, the relaxation of a proton can be significantly enhanced by a nearby quadrupolar nucleus via magnetic dipole coupling, if their transition frequencies match. In principle, this effect can be used to enhance image contrast in MRI in a frequency selective manner². As a first promising guess, Bi-aryl compounds seem to be suitable as a starting point for designing a novel contrast agent based on the QRE effect and to tune it for applications on a 3 T scanner.

NQR Spectroscopy is a chemically and structurally very sensitive spectroscopy method that is probing high spin ($I > 1/2$) nuclei in solid samples without the need of an external magnetic field. Using RF pulse sequences, the technique has the potential to fully determine the transitions of a spin ensemble regarding their relaxation properties. Also, the spatial symmetry and the quadrupolar coupling strength of the intramolecular electric field gradient at the position of the probed nucleus can be derived experimentally; these parameters determine the frequency positions of the nuclei's spin transitions.

Method

NQRS experiments are carried out using two complementary RF-pulse spectrometer systems; the self-constructed „ConCradle” and the commercial system „Scout” from Tecmag, Inc. (Texas). The available RF coils cover a range of 20 MHz up to 150 MHz and can be thermalized around body temperature or in liquid nitrogen. Both systems are placed in a shielding chamber to protect the measurements from RF spur signals. For T_1 and T_2 relaxation time measurements pulse sequences well known in the NMR community are used, as for example spin echo and inversion recovery.

Results and discussion

The nuclear quadrupole spin transitions of six Bi-aryl derivatives with different substituents and their corresponding relaxation times (T_1 and T_2) at 37 °C body temperature and liquid nitrogen temperature have been determined. From the transition frequencies their NQR parameter-Quadrupole Coupling Constant Q_{cc} and asymmetry parameter η - are calculated.

As Bi has nuclear spin 9/2, there are four spin transitions where so far only three for each sample could be identified.

The results show the tuning possibilities of NQR transition frequency positions and their relaxation behaviour by the targeted use of substituents on molecules.

[1] D. Kruk et. al., *Solid State Nuclear Magnetic Resonance*, 40 (2011) 114-120

[2] D. J. Lurie et. al., *Comptes Rendus Phys.*, Bd. 11, Nr. 2 (2010) 136-148