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POSTERS ABSTRACT BOOK

OTH-007: NMR Relaxation by Redfield equation in a spin system I=7/2

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Introduction

The Redfield theory is an approach that allows us to describe the relaxation theory by applying quantum mechanics concepts and exploring the density matrix definition [1, 2]. Consequently, all the coherence orders can be determined analytically or numerically. Additionally, the number of relaxation rate constants established by Tsoref-Eliav-Navon et al. [3] was extended, and mathematical expressions were established for the longitudinal and transverse magnetization.

Aims

The Redfield theory must be applied to determine the analytical (order coherence 7,...,2) and numerical (order coherence 1 and 0) solutions for all the density matrix elements of an isolated spin 7/2 system.

Methods

Our research involved two NMR experiments, the spin-echo and inversion-recovery, conducted in a lyotropic liquid crystal Cs-PFO. The characteristic seven spectral lines of a spin 7/2 nuclei were monitored to measure the longitudinal and transverse magnetization in static magnetic field strength of 9.4 Tesla.

Results

All the relaxation rate constants that determine the dynamics of the spin 7/2 system were accurately characterized. This precision in characterizing the dynamics allows us to find the spectral density values and test the theoretical solutions. The amplitudes predicted by the theory were compared with the Laplace Transform tool and the values are remarkably close, further validating the accuracy of our theoretical predictions.

Conclusions

Using the model developed in this work, the theoretical result allows us to describe any spin system 7/2 isolated.

References

- [1] Redfield, Alfred G. On the theory of relaxation processes. IBM Journal of Research and Development. 1957, 1, 19-31.
- [2] A. Consuelo-Leal, et al. NMR Relaxation by Redfield equation in a spin system I= 7/2. Journal of Magnetic Resonance, v. 349, p. 107403, 2023.
- [3] Tsoref, L., U. Eliav, and G. Navon. Multiple quantum filtered nuclear magnetic resonance spectroscopy of spin 7/2 nuclei in solution. The Journal of chemical physics, 1996.