Coordination Complexes for Spin-Based Quantum Computation

M.J. Graham (Northwestern U., Chemistry); M. Shiddiq (FSU, Physics); S. Hill (NHMFL and FSU, Physics); D.E. Freedman (Northwestern U., Chemistry)

Introduction

Quantum computation is an information processing technique that exploits the unique properties of quantum mechanical systems. One paradigm that has been proposed for the physical implementation of a quantum computer employs electronic spins in paramagnetic coordination complexes [1]. In evaluating candidate complexes to host electronic spin-based qubits, the most important metric is the coherence time, which is equal to the transverse relaxation time of the complex as measured by pulsed EMR spectroscopy.

Though numerous relaxation studies of individual complexes have been reported, no study has ever systematically and experimentally examined the dependence of the transverse relaxation time on modifiable chemical properties like spin, spin-orbit coupling, and proximity/type of nuclear spins in the paramagnetic complex. We set out to perform such a study by examining a series of monometallic, octahedral coordination complexes.

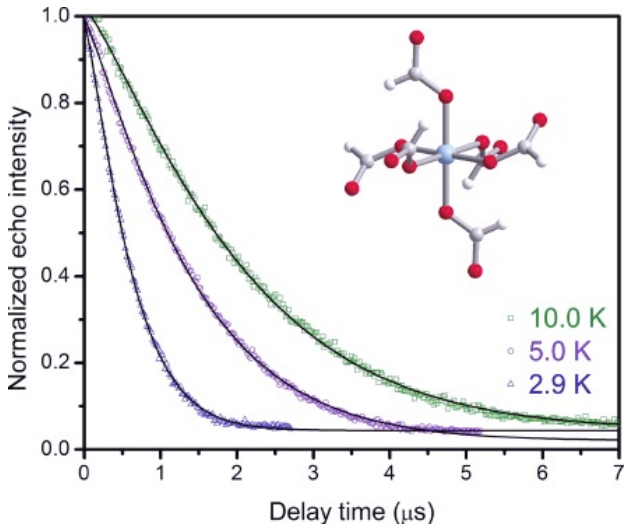

Figure 1. Transverse relaxation data for $K_3Cr(HCO_2)_6$.

Experimental

Relaxation data were taken at the Tallahassee NHMFL campus in the EMR group on both a Bruker E680 X-band spectrometer and a 240 GHz heterodyne spectrometer. CW spectra were obtained on a broadband transmission spectrometer in order to obtain values of *D*. Solutions were measured in a frozen solution of 1:1 water/glycerol at concentrations ranging from 0.1 to 10 mM.

Results and Discussion

The obtained relaxation data indicate that spin-orbit coupling plays a significant role in determining the overall relaxation time, even at extremely low temperatures. This is unexpected, as spin-orbit coupling affects transverse relaxation via the longitudinal relaxation, T_1, which is extremely slow at low temperatures. Additional experiments elucidated the dependence of relaxation time on spin, and showed that increasing the spin of a complex from S = 3/2 to S = 5/2 increased the relaxation time by 50%. Preliminary data were taken to examine the dependence of the relaxation time on the magnitude and proximity of nuclear spins in the ligand field, and indicated a complicated relationship that warrants further study.

Conclusions

A series of relaxation studies were performed to examine the effects of electronic spin magnitude, nuclear spin proximity and magnitude, and spin-orbit coupling on the transverse relaxation of paramagnetic coordination complexes. The studies illustrated the significance of spin-orbit coupling as a contributing factor to relaxation and showed evidence of a complicated dependence of relaxation on nuclear spin.

Acknowledgements

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References

[1] Leuenberger, M.N., *et al*., Nature, **410**, 789–793 (2001).