SPIN RELAXATION OF DECAMETHYLFERRICINIUM

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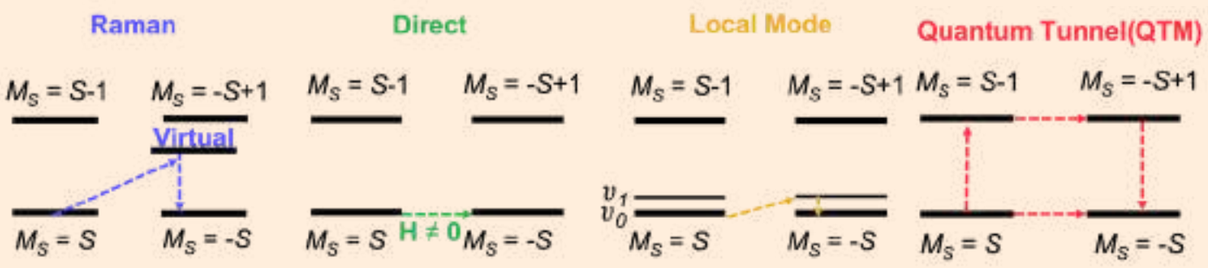
BACKGROUND

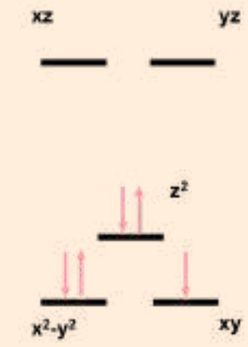
QUBITS

Molecules with long coherence times and the ability to compete with NV centers are under investigation.

There are different spin relaxation mechanisms for this system:

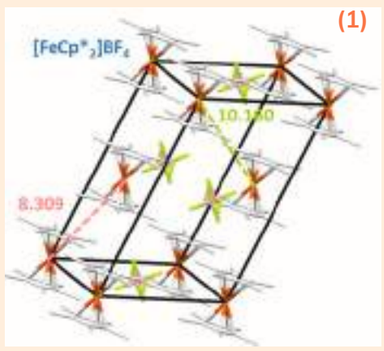


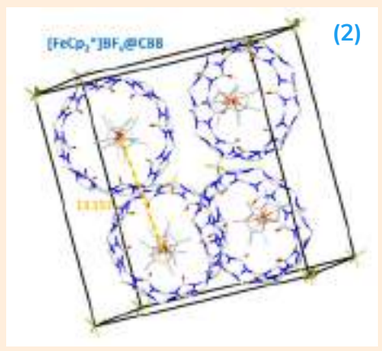
Iron metallocenes with S=1/2 show considerable axial anisotropy due to their fundamental states. with a Non-Aufbau occupancy. However, they exhibit fast magnetic relaxation induced by the quantum tunnelling that it is promoted by intermolecular dipolar interactions.



HOW TO AVOID IT?

A rigid environment can modify the vibrations of the molecule and decrease dipolar interactions. The encapsulation in cucurbit[8]uril is presented.





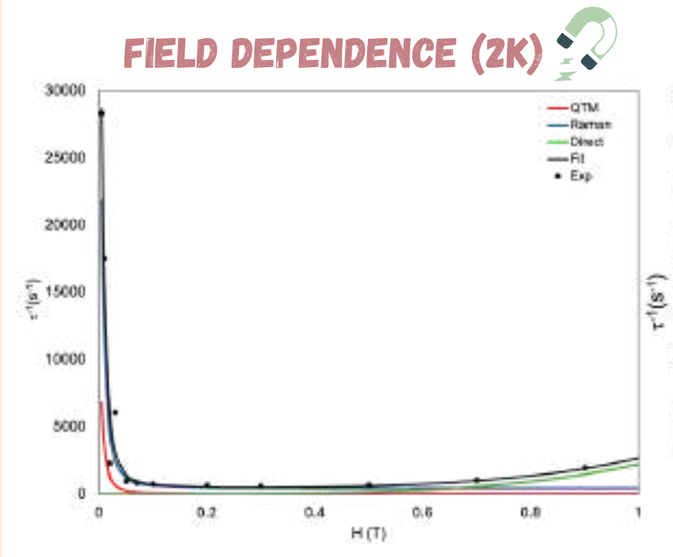
RESULTS

SQUID RESULTS

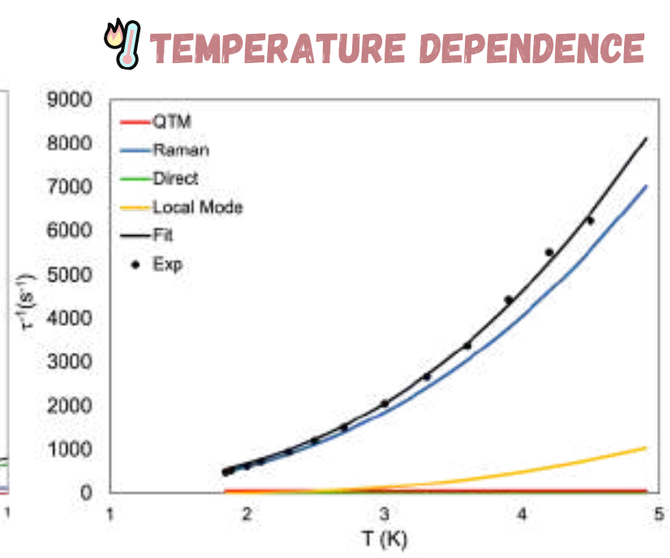
$$\tau^{-1} = \frac{1+eH^2}{1+fH^2} dT^n + AH^4T + C_{loc}\frac{\exp(\Delta_{loc}/T)}{(\exp(\Delta_{loc}/T)-1)^2} + \frac{B_1}{1+B_2H^2}$$

Raman Direct Local Mode QTM

FIELD DEPENDENCE (2K)



TEMPERATURE DEPENDENCE

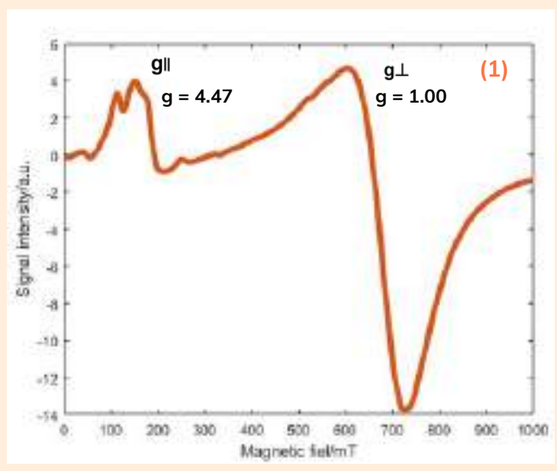


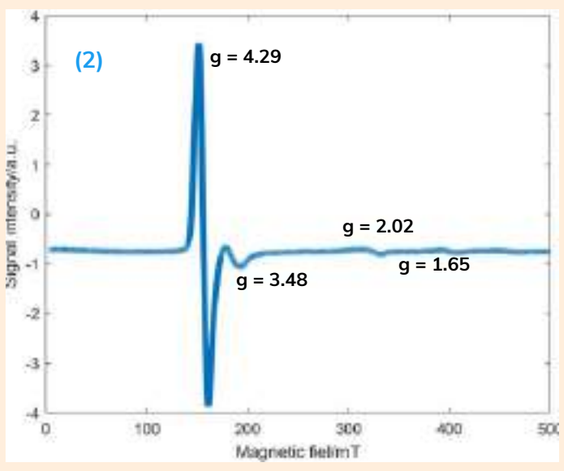
The spin relaxation mechanisms studied by analyzing the **depedence with the field** where the Raman term is the one that governs the relaxation- At low fields QTM term has reduce . At high fields is controlled by Direct term.

The spin relaxation mechanism studied by analyzing the **dependence with the temperature** where the predominant term in all the regions is Raman and at high temperatures is slightly influence by Local Mode.

EPR RESULTS

CONTINUOUS WAVE (CW)

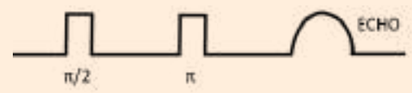




Not easy assignment of g values, work in progress.

EPR SEQUENCES

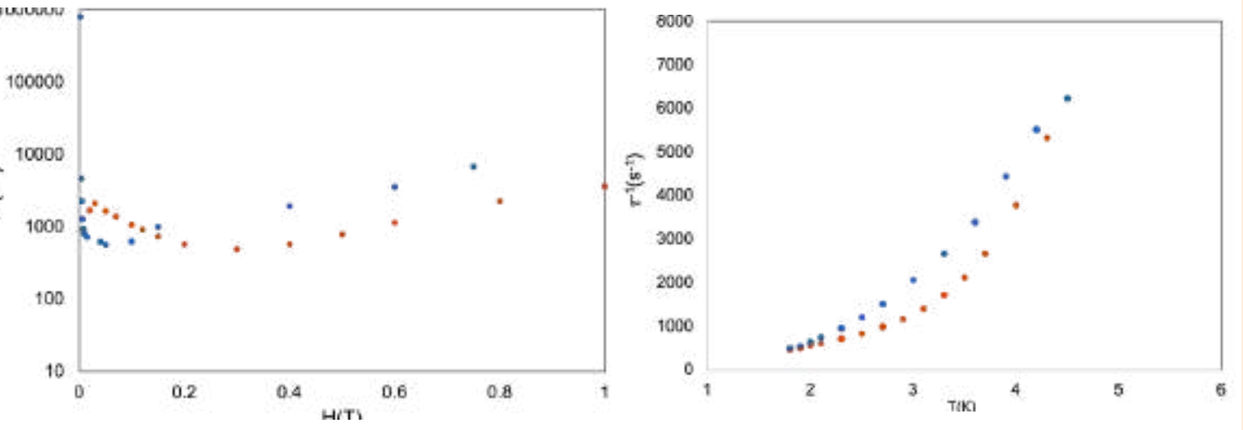
Hahn-echo (T2)

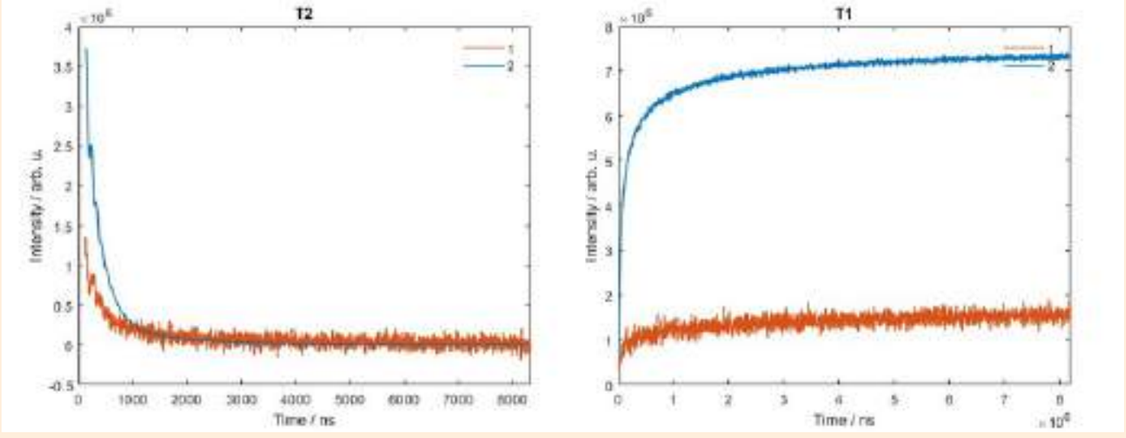


Inversion Recovery (T1)

HOW DOES ENCAPSULATION IMPROVE RELAXATION TIME?

Preliminary EPR results at 3K.





The relaxation time measured on the Squid corresponds to the T1 measured on the EPR.

With the encapsulation, the **dipole interactions decrease** and consequently the **relaxation time increases**, favouring other relaxation mechanisms.

REFERENCES

[1] D. Aravena, E. Ruiz. Dalt. Trans. 2020, 49, 9916-9928.
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FUTURE PROYECTS

- Magnetic dilution of the above system.
- Find out the relaxation mechanisms of the above system with EPR measurements at different temperatures.
- Continue with the characterization of decamethylferrocenium in another organic host.