A CHEMIST'S TOOLBOX TO TUNE 4F MOLECULAR QUBITS

Christian D. Buch[a], Steen H. Hansen[a], Anton Viborg[a], Jonatan B. Petersen[b], Richard Winpenny[b], and Stergios Piligkos[a]

[a]Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark
[b]School of Chemistry, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

Quantum computers are going to have a transformative impact on our society, promising to be tremendously faster than any classical computer of today in several areas e.g. database search and simulating biomolecules. These computers are based on the quantum bit (qubit) which is a two-level system that cannot only assume the states |0> or |1> but also any arbitrary superposition of these. Many systems are investigated as qubits including superconductors, molecular systems, photons and nitrogen-vacancies in diamonds. The advantage of molecular systems is that they can be chemically tuned. Changing the molecular backbone of the qubit its static and dynamic quantum properties can be modified. Although much emphasis is placed on the tunability of molecular qubits, there exists very few studies that systematically investigate how molecular systems can be tuned by introducing new chemical groups or changing the position of chemical groups within the molecule.

Recently, we have studied Gd(trensal) and Yb(trensal) (Figure 1) as molecular qubit candidates, finding phase memory times of up to 12 µs at 3 K.[1, 2] Herein, we present how the introduction of various chemical groups, such as methoxy groups (Figure 1, left) and formyl groups, to the Ln(trensal) ligand scaffold influences the static and dynamic spin properties of the Ln(trensal) systems. Additionally, the position of these new groups on the phenyl rings is investigated as an additional way of tuning the systems (Figure 1, right).

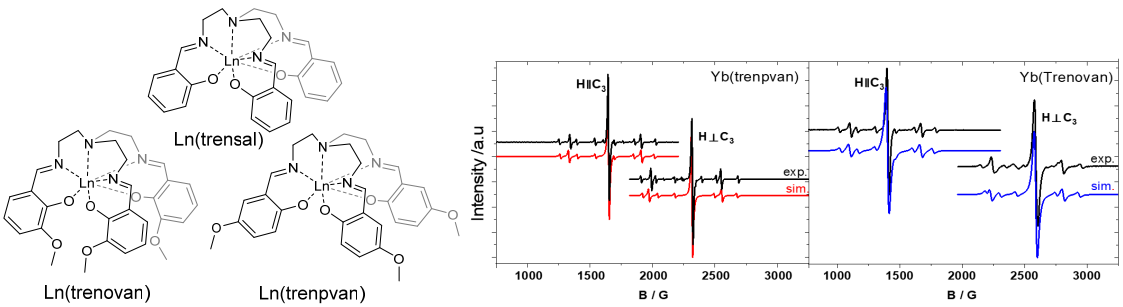

Figure 1. *Left*: Structures of Ln(trensal) and its methoxy derivatives Ln(trenovan) and Ln(trenpvan). *Right*: Single crystal c.w.-EPR spectra of Yb(trenovan) and Yb(trenpvan).

[1] Buch, C. D. et al., *JACS*, **2022**, 144, 17597-17603

[2] Pedersen, K.S. et al., *JACS*, **2016**, 138, 5801-5804