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"Fun with lanthanide ligand fields"

Abstract. Molecular systems which display the ability to retain magnetisation, in the absence of an external magnetic field, resulting in the appearance of magnetic memory of molecular origin, are known as Single-Molecule Magnets (SMMs).[1] In 4f-SMMs, the energy barrier to reorientation of the magnetisation (U_{eff}) is strongly determined by the control of the coordination environment at the lanthanide centre. Synthetic chemists have been guided by the predictions of many computational research groups based on *ab initio* calculations.[2-4] Specifically, the use of dysprosium(III) in targeted coordination environments that promote strong uniaxial symmetry stabilizes the largest m_J = ±15/2 ground state and gives large U_{eff} barriers.[5]

In the first part of the lecture, I will show how this can be achieved by using macrocyclic or polydentate ligands by careful tuning of the axial and equatorial ligand fields.[6-9] In the second part of the lecture, I will focus on holmium(III), again in a targeted coordination environment, but instead of SMM properties I will show how we can engineer spin clock transitions.[10-11] This a new area when applied to molecular complexes, with the goal of developing molecular spin qubits with built-in protection against unwanted sources of magnetic noise.

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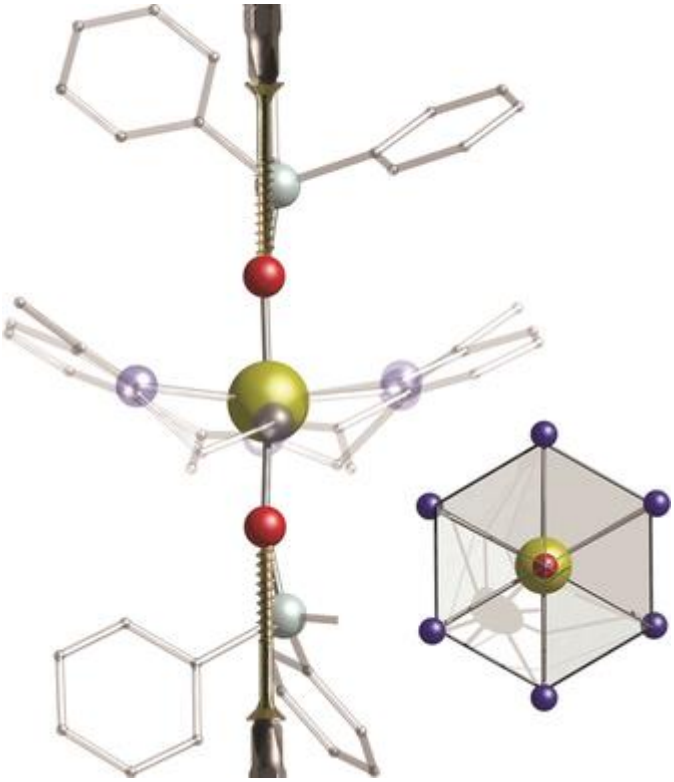

Figure: Combining a strong linear axial ligand field with a weak equatorial ligand field.