

Neutron and x-ray diffraction studies of magnetic anisotropy in single molecule magnets

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Single-molecule magnets are a fascinating type of compounds that, after being magnetized by an external magnetic field, can keep their magnetization for prolonged periods of time. This property arises due to the ordering of states in molecules with unpaired electrons and is manifested in anisotropy in parameters such as the zero-field splitting, the g-tensor and thus the magnetic susceptibility. In this seminar, I will introduce the concept of molecular magnetism and present two techniques we use for studying it: one is multipole modelling of x-ray diffraction patterns to determine molecular charge densities, which we correlate with magnetic properties. The other method, polarized neutron diffraction, is used for modelling the degree and the direction of the molecular magnetic anisotropy. Both techniques provide important experimental clues to the relationship between molecular structure and magnetic anisotropy, which can be used to guide both the development of theory and the targeted synthesis of new compounds.