# Investigation of the viability of structural information determined with X-ray diffraction employed to determine anisotropic magnetic susceptibility

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Single molecule magnets (SMM) are an interesting topic within the domain of materials chemistry, with possible uses for quantum computing and high density data storage. This study is concerned with the use of polarized neutron diffraction (PND) to describe them.

If a SMM crystal sample is measured with a classical magnetometer, it would yield a simple vector sum of all site magnetizations in the crystal. To access the anisotropic magnetic susceptibility tensor of the individual sites, (PND) can be used. Neutrons will scatter as a result of both the magnetic and the nuclear strong force interaction. In a (PND) experiment we measure the combined diffraction pattern from both interactions, but want to isolate the magnetic part in order to calculate the anisotropic susceptibility tensor. I.e. we need to find the contribution from nuclear strong force separately, which can be calculated from the crystal structure. The structure is usually found using unpolarized neutron diffraction, as opposed to XRD because of the importance of scattering from light elements. However neutron diffraction experiments are significantly harder to come by, this study has investigated the effect of using a high quality XRD structure as a basis instead.

Two known molecular magnets, have been investigated: One with a Co(II) and one with a Dy(III) ion core. For both systems, susceptibility tensors are refined using both a neutron diffraction structure and different X-ray diffraction structures. The X-ray results are compared to the neutron tensor to gauge the impact on the refinement. Ultimately the goal is to decide if X-ray diffraction could be considered as a substitute for neutron diffraction when solving the crystal structure of a molecule with the aim of finding the magnetic susceptibility.

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