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Polarized Neutron Diffraction study of the molecular magnetic anisotropy

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The magnetic anisotropy is a prerequisite for a metal complex to behave as a single-molecule magnet (SMM). Unfortunately, today we do not fully understand the relationships between the local structural parameters and the magnetic anisotropy that results at the molecular level. This is an issue that has become recursive in this area. Out of the synthesis work which is still important, but generates a multiplication of SMMs with frustrating properties, there are various studies to understand these relationships among which most are theoretical studies. In this context, we believe that polarized neutron diffraction (PND) can provide an experimental and complementary point of view to these theoretical studies. PND is indeed well known to allow an accurate determination of the spin density in magnetic compounds and in the field of molecular magnetism it has provided unique information on the pathways and the nature of intra- or intermolecular magnetic coupling [1]. In the case of highly anisotropic paramagnetic materials, where local magnetic moments cannot be aligned by an external magnetic field, that is more tricky, but a method based on local magnetic susceptibility tensor, has been recently developed that allows now analysing the data in this case and obtaining the magnetization distribution [2]. This approach was first used for inorganic compounds. Our idea has been to use this approach to go beyond the reconstruction of spin density to study the magnetic anisotropy in molecular systems. In this paper, we present the results of such an approach applied for the first time to metal complexes that are simple mono and dinuclear cobalt(II) complexes.

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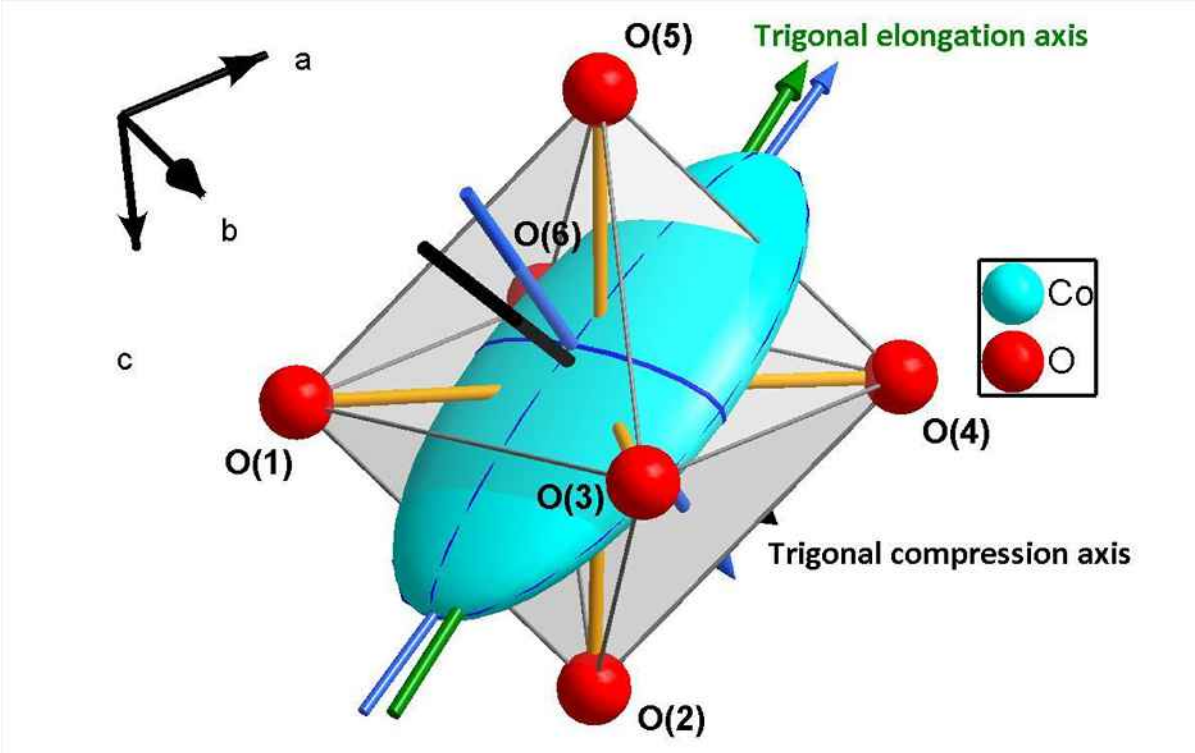

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