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Multi-Technique Experimental Benchmarking of the Local Magnetic Anisotropy of a Cobalt(II) Single-Ion Magnet

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A comprehensive understanding of the ligand field and its influence on the degeneracy and population of d-orbitals in a specific coordination environment are crucial for the rational design and enhancement of magnetic anisotropy of single-ion magnets (SIMs). Herein, we report the synthesis and comprehensive magnetic characterization of a highly anisotropic Co^{II} SIM, $[L_2Co](TBA)_2$ (L is an N,N -chelating oxanilido ligand), that is stable under ambient conditions. Dynamic magnetization measurements show that this SIM exhibits a large energy barrier to spin reversal $U_{eff} > 300K$ and magnetic blocking up to 3.5 K, and the property is retained in a frozen solution. Low-temperature single-crystal synchrotron X-ray diffraction used to determine the experimental electron density gave access to Co d-orbital populations and a derived U_{eff}, $261cm^{-1}$, when the coupling between the $d_{x^2-y^2}$ and d_{xy} orbitals is taken into account, in very good agreement with ab initio calculations and superconducting quantum interference device results. Powder and single-crystal polarized neutron diffraction (PNPD, PND) have been used to quantify the magnetic anisotropy via the atomic susceptibility tensor, revealing that the easy axis of magnetization is pointing along the N–Co–N′ bisectors of the N,N′-chelating ligands (3.4° offset), close to the molecular axis, in good agreement with complete active space self-consistent field/N-electron valence perturbation theory to second order ab initio calculations. This study provides benchmarking for two methods, PNPD and single-crystal PND, on the same 3d SIM, and key benchmarking for current theoretical methods to determine local magnetic anisotropy parameters.

The results of the work are published in [1].

1. S.K.Gupta, H.H.Nielse, A.M.Thiel et al. JACS Au 2023, 3, 429–44

Primary author: KIBALIN, Iurii (ILL)

Presenter: KIBALIN, Iurii (ILL)

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