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Crystal structures and cryomagnetic studies of Sm^{3+} and Ho^{3+}, Yb^{3+} complexes as potential candidates for quantum technologies

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Lanthanide complexes are very versatile in their applications in fields of knowledge such as biomedicine, high-density information storage, quantum processing information, and spintronics.[1] In this work, we investigate the use of the (2,4,6-trimethylphenyl)oxamate ligand[2] (2,4,6-tmpa), and Sm^{3+} and Ho^{3+} to synthesize new inclusion complexes of general formula *n*-Bu_4N[Ln(2,4,6-tmpa)$_4$(H_2O)]·1.5H_2O·3DMSO, where Ln = Sm^{3+} (**1**) and Ho^{3+} (**2**), and Yb^{3+} (**3**) *n*-Bu_4N[Yb(2,4,6-tmpa)$_4$]·1.38H_2O·0.62DMSO·[*n*-Bu_4N is tetrabutylammonium and DMSO is dimethylsulfoxide]. All complexes were characterized by thermogravimetry, elemental analysis, IR spectroscopy, and X-ray powder diffraction patterns (PXRD). Their crystal structures were determined by single-crystal X-ray diffraction (SCXRD). The anionic part comprises four 2,4,6-tmpa ligands, one water molecule of coordination for **1** and **2**. Magnetic measurements in both static direct current (dc) and dynamic alternating current (ac) were measured in polycrystalline samples. The data suggested that **1** is weakly paramagnetic and **2** shows no slow magnetic relaxation. At the same time, **3** presented the slow relaxation of the magnetization phenomena, making it single-ion magnet and potential candidate as spin qubits for quantum computing at low temperatures.[3]

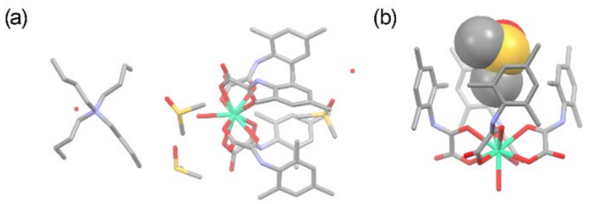

Figure 1. (a) Representation of crystal structure of **1** (view along the *a* axis); (b) anionic part of the inclusion complex (view along the *c* axis). Color codes: C, gray; oxygen, red; sulfur, yellow; nitrogen, light blue. Hydrogen atoms were omitted for the sake of clarity.

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