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Synthesis and characterization of a new Fe_3-Re_6 oxo-bridged polyheteronuclear complex

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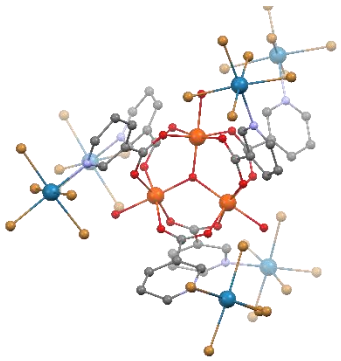
Molecular magnetism is an active area of research that has historically benefited from several subareas of chemistry and physics, such as coordination and supramolecular chemistry, solid-state physics, theoretical, and computational chemistry and crystallography, among others. Nevertheless, research has focused chiefly on 3*d* and 4*f* metal complexes, leaving out interesting 4*d* and 5*d* metals as possible spin carriers.[1,2] In this regard, rhenium(IV) presents itself as an attractive choice among the heavy transition elements due to its S = 3/2 spin configuration and its high spin-orbit coupling constant that makes rhenium(IV) complexes have high magnetic anisotropy of the ground state.[3]
Herein, we present preliminary results on the synthesis and characterization of a new rhenium(IV)-iron(III) complex (**1**) of formula $(NBu_4)_2\{Fe_3O(H_2O)_3[ReBr_5(nic)]_3[ReBr_5(Hnic)]_3]\}\cdot 2^iPrOH$ (NBu_4 = tetrabutylammonium; Hnic = nicotinic acid; ^{i}PrOH = isopropanol). The crystal structure of the complex was determined, showing that the nonanuclear anionic units adopt a triangular oxocentric Fe_3O motif in which each pair of iron(III) ions are bridged together by two carboxylate groups from the rhenium metalloligands, with two tetrabutylammonium cations as counterions. The magnetic properties of the compound were studied on microcrystalline samples from 2 – 300 K via *ac* and *dc* susceptibility measurements.



Topside view of the nonanuclear complex 1 to make easier the visualization of the central $[Fe_3O(RCOO)_6]^+$ unit. Color code: red (O), orange (Fe), yellow (Br), blue (Re), purple (N), grey (C). Tetrabutylammonium counterions, hydrogen atoms, and solvent molecules are omitted for clarity.

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