Title:	Fe6 clusters of tripodal alcohol ligands: Synthesis, structures and magnetostructural properties
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Abstract:	The synthesis, crystal structures, cyclic voltammetric and magnetic characterization of (NEt3H)2[FeIII6Cl6(μ6-O)(thme)4]·3(H2O) (1) (H3thme = trishydroxymethyl ethane) and (NEt3H)2[FeIII6Cl6(μ6-O)(thmp)4]·5.5(H2O) (2) (H3thmp = trishydroxymethyl propane) are reported. Both complexes crystallized in the orthorhombic system and have the space group Pca21. The metallic cores of the complexes comprise of the [(μ6-O)Fe6(μ-O)12] unit. The ligands thme3− and thmp3− adopt the same η2, η2, η2, μ3-bridging mode of the alkoxide oxygen atoms in 1 and 2. Electrochemical studies are consistent with formation of stable quasi-reversible one electron FeII/III redox couples in solution. The fascinating features of the non-covalent supramolecular contacts have been explored and corroborated theoretically by Hirshfeld surface analysis along with electrostatic potential (ESP), deformation density (DD) and ab initio calculations. The interplay of the interactions, (i.e., H···O, Cl···H and other contacts) give rise to the consolidation of discrete units of 1 and 2 into supramolecular architectures. Variable-temperature and field (H) solid-state direct and alternating current magnetic susceptibility measurements were done on samples of 1 and 2 in the temperature range 1.8–300 K. Analysis of the data confirmed the presence of dominant antiferromagnetic interactions, leading to an S = 0 ground state, and no out of phase ac magnetic susceptibility signals were observed for either cluster, ruling out single-molecule magnet behaviour.
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