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Title:	Synthesis, structural characterization and Csingle bondH activation property of a tetra-iron(III) cluster
Authors:	Dey, D. (/jspui/browse?type=author&value=Dey%2C+D.) Yadav, H.R. (/jspui/browse?type=author&value=Yadav%2C+H.R.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Iron Bridging ligand X-ray crystal structure Magnetic property
Issue Date:	2019
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Citation:	Journal of Molecular Structure, 1180, pp. 220-226.
Abstract:	A non-heme tetra-iron cluster, [Fe ₄ III(μ-O) ₂ (μ-OAc) ₆ (2,2'-bpy) ₂ (H ₂ O) ₂](NO ₃ ⁻)(OH ⁻) (1), [OAc = acetate; 2,2'-bpy = 2,2'-bipyridine] containing oxido- and acetato-bridges was synthesized and structurally characterized by different spectroscopic methods including single crystal X-ray diffraction studies. X-ray crystal structure analysis of 1 revealed that tetra-iron complex was crystallized in monoclinic system with C2/c space group. Each of the Fe centres in 1 was found to exist in octahedral geometry and interconnected by oxido- and acetato-bridges. Bond valence sum (BVS) calculation recommended the existence of iron centres in +3 oxidation state. Variable temperature magnetic measurement authenticated the dominating antiferromagnetic ordering among the iron centres in the solid state of 1. This tetra-iron cluster was also evaluated as an efficient catalytic system towards the oxidation of both linear & cyclic alkanes without production of primary Csingle bondH bond oxidation products. Oxidation of secondary Csingle bondH bonds attested the formation of both the corresponding alcohols & ketones in 27–900 TONs. The tetra-iron catalytic system with Alcohol/Ketone values 0.2–1.7 indicated the involvement of freely diffusing carbon-centered radicals rather than metal based oxidant.
Description:	Only IISERM authors are available in the record.
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