

IRON(III) CLUSTERS WITH 3-FORMYLSALICYLIC ACID

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In the presence of additional ligands and polar solvents, the well-known μ_3 -OXO bridged triangular iron carboxylates easily reorganize and stabilize large complexes. We chose 3-formylsalicylic acid (H₂L) in order to explore its coordinative ability, due to its multiple coordination donor groups like –COOH, –OH and –CHO. Herein, new hexanuclear iron(III) clusters [Fe₆O₂(OH)₂(L)₂(H₂O)₂(O₂CR)₈]·MeCN (R = CMe₃ (**1**); CHMe₂ (**2**)), where L is the dianion of 3-formylsalicylic acid, are reported. Compounds **1** and **2** were prepared from the reaction of μ_3 -oxo trinuclear iron(III) precursors [Fe₃(μ_3 -O)(H₂O)₃(O₂CR)₆(O₂CR)·2HO₂CR with 3-formylsalicylic acid in acetonitrile. Both structures comprise six Fe atoms in an almost planar arrangement that can be described as two oxo-centered triangular units [Fe₃(μ_3 -O)]⁷⁺ joined together by two bridging hydroxide and two bridging carboxylate groups. The asymmetric units contain only half of an Fe₆ molecule. All Fe atoms adopt distorted octahedral coordination geometries and are in the +3 oxidation state. The peripheral ligation of metal ions is completed by six carboxylate molecules and two aldehyde ligands which are in their monoanionic and dianionic forms, respectively. The two 3-formylsalicylic ligands act as tridentate, bridging Fe1 (Fe1') and Fe2 (Fe2') ions by the alkoxo groups within each [Fe₃(μ_3 -O)]⁷⁺ unit. The oxygen atom of the formyl group is also coordinated, which was not reported so far for this ligand. All carboxylate groups adopt the bridging μ_2 - η^1 : η^1 coordination mode: two of them join the edges of the triangular [Fe₃(μ_3 -O)]⁷⁺ units and the remaining six link Fe atoms within the latter (Fig. 1). Detailed characterization of compounds **1** and **2** will be described in a forthcoming paper.

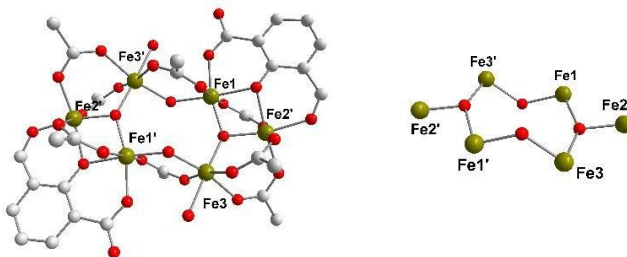


Figure 1. The molecular structure of complex **2**·CH₃CN (left) and its [Fe₆(μ_3 -O)₂(μ -OH)₂]¹²⁺ structural core (right).

Color code: Fe^{III}, olive green; O, red; C, grey. The hydrogen atoms, methyl groups and solvent molecules are omitted for clarity.

Keywords: 3-formylsalicylic acid, asymmetric units, hexanuclear iron(III) clusters, peripheral ligation.