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A novel binuclear Mn(III) tridentate schiff base complex [C₂₂H₂₆Cl₄Mn₂N₂O₆] (1) has been synthesized and its crystal structure has been determined by single crystal X-ray diffraction analysis. Structural analysis shows that the Schiff base ligand of this dimeric Mn(III) complex coordinates toward one Manganese atom in a tridentate mode and each Mn atom is six-coordinated. Magnetic susceptibilities for (1) in the solid state have been measured over the temperature range 2-350 K as a function of temperature and the magnetic parameters have been determined with fitting procedure. Magnetic measurements on (1) reveal the presence of antiferromagnetic spin-exchange interactions between the manganese(III) ions.

Keywords: ONO donors, Binuclear Mn (III) complexes, X-ray crystallography, Magnetic exchange

FA4-MS34-P36

The hexadecaioiodide Ion I₁₆²⁻. Synthesis and crystal structure of [Na(15c5)]₂I₁₆. Ingo Pantenburg,

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The hexadecaioiodide ion is one of the most iodine rich polyiodide described in the literature. The tendency to decompose and to emit iodine is large and, therefore, hexadecaioiodides are rather elusive. However, bulky cations with a low and shielded charge are able to stabilize even such a large polyiodide anion [1].

Two heptaioiodide anions are linked by an iodine molecule to form the hexadecaioiodide in [Na(15c5)]₂I₁₆ (1). The crystal structure of 1 contains the dimeric in-cavity-complex [Na(15c5)]₂²⁺. The sodium atoms Na1 and Na2 are located 62 pm above the average plane through the oxygen atoms of the crown ether ligand. Both complex sodium ions dimerize through the μ-bridging oxygen atoms O101 and O204 of the crown ether (d(Na1-Na2) = 342.9(9) pm; see Fig. 1, left).

The charge-compensating hexadecaioiodide I₁₆²⁻ in 1 is built up by two pyramidal heptaioiodide ions, which are linked to each other through the terminal iodine atoms I113 and I213 by the iodine molecule I241-I242 resulting in the configuration [I₇·(I₂)·I₇] (d(I113-I242) = 348(1), d(I213-I241) = 347(1) pm). The heptaioiodide ions themselves are made up by one asymmetric almost linear triiodide anion (d(I111-I112-I113) = 296.3(9), 286.8(9), d(I211-I212-I213) = 295.5(8), 287.2(8) pm) connected to two iodine molecules with the configuration [I₃·2(I₂)]. In the crystal structure, the hexadecaioiodide ions form chains along the *a*-axis (d(I113-I132) = 346(2), d(I213-I222) = 342(2) pm; see Fig. 1, right).

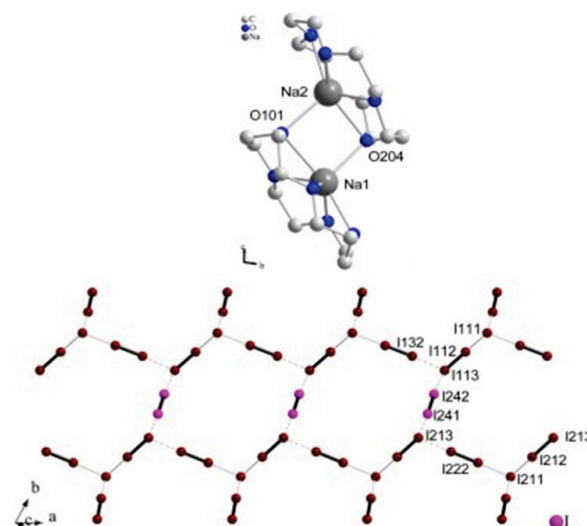


Fig. 1. The dimeric in-cavity-complex [Na(15c5)]₂²⁺ (top) and the anionic I₁₆²⁻ chain (bottom).

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Keywords: Polyiodides, Crown Ether, Crystal Structure

FA4-MS34-P37

Two novel scandium croconate and mixed croconate-oxalate complexes. Celeste Bernini^{a, b}, Natalia Snejko^a, Marta Iglesias^a, Enrique Gutierrez-Puebla^a, M Angeles Monge^a, ^aInstituto de Ciencia de Materiales de Madrid, CSIC, Spain, ^bArea de Química General e Inorgánica, Universidad Nacional de San Luis, Argentina.

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Polynuclear complexes feature a fascinating variety of unusual symmetries and structural patterns

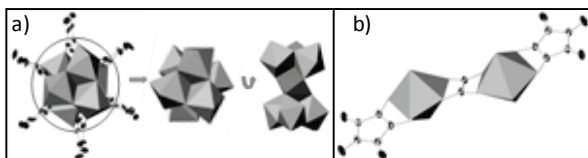
[1]. On the other hand, the synthesis of inorganic clusters continues attracting considerable attention, due to the interesting properties of the metallic aggregates[2]. The control of the lanthanide ions hydrolysis in presence of appropriate ligands appears as a common strategy to obtain the hydroxo REE clusters[3].

It is a known fact that the Sc(III) ion is a good Lewis acid and is currently used to prepared stable complexes and MOFs, because such compounds find application in homogeneous and heterogeneous catalysis[4]. The croconate, a cyclic oxocarbon dianion, is a member of the (C_nO_n)₂- series composed by the deltatate, squarate, croconate and rhodizonate anions, with n = 3-6, respectively. Some of these oxocarbon anions can suffer oxidation. Such process has been observed for squarate oxidized into oxalate in lanthanide oxalate-squarate compounds[5], and in calcium croconate-oxalate complexes[6]. With this in mind, we set the challenge of controlling the synthesis conditions in order to obtain compounds with croconate as the only ligand and another that contain the croconate and the oxalate ions in the same framework. Here we present two Sc(III) complexes based in croconate and mixed croconate-oxalate ligands, with formulas [Sc7(C5O5)6(OH)7(H2O)6O], Figure 1a, and

[Sc₂(crocn)₂(ox)₂(H₂O)₆]₂•2.5H₂O, Figure 1b. Also we report the results in the catalytic activity tests in acetalization and cyanosilylation of benzaldehyde.

Figure 1: a) [Sc₇(C₅O₅)₆(OH)₇(H₂O)₆O], b) [Sc₂(crocn)₂(ox)₂(H₂O)₆]₂•2.5H₂O.

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Keywords: Scandium, croconate, heterogeneous catalyst