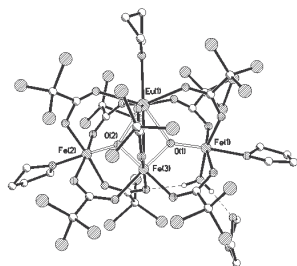


s13.m35.p22 **From μ_3 -Oxo-Bridged Trinuclear Clusters to the Tetranuclear 4f-3d Carboxylate System Containing $[4fFe_3O_2]^{8+}$ Core.** Sergiu Shova^a, Constantin Turta^b, Yurii A. Simonov^a, Maria Gdaniec^c, Denis Prodius^b, Valeriu Mereacre^b, ^aInstitute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova, ^bInstitute of Chemistry of the Academy of Sciences of Moldova, Chisinau, Moldova, ^cFaculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780, Poznan, Poland. Email: shova@usm.md

Keywords: Heterocluster; Structure; Ferromagnetic interaction

Oxo-centered carboxylate-bridged trinuclear complexes of the general formula $[Fe_2MO(RCOO)_6L_3]X_n \cdot (Solv.)_m$ are known for a wide variety of bridging carboxylate anions (RCOO), monodentate terminal ligands (L), and M = 3d-elements or Fe²⁺. The molecular heterometallic iron-containing trinuclear carboxylates attract a special attention. A considerable number of such type of complexes that incorporate heterometallic $[Fe_2VO]^{6+}$, $[Fe_2CrO]^{7+}$, $[Fe_2MnO]^{6+}$, $[Fe_2CoO]^{6+}$, $[Fe_2NiO]^{6+}$, $[Fe_2ZnO]^{6+}$ or homometallic mixed-valence $[Fe_2FeO]^{6+}$ cores, has been recently studied by X-ray method. This presentation includes the results of synthesis and X-ray single-crystal investigation for a series of novel mixed-metal and mixed-valence trinuclear iron carboxylates with discernable localization of the hetero-metal positions in μ_3 -oxo-centered trinuclear core. The complexes under discussion are divided into several groups where the metals used are characterized by a) close values of atomic numbers, and essentially different coordination environment, $[Fe_2MnO(CHCl_2COO)_6(THF)_2 \cdot H_2O]$; b) essentially different atomic numbers and the same coordination environment, $[Fe_2MgO(CCl_3COO)_6(Py)_3] \cdot CH_3C_6H_5$, $[Fe_2MgO(CCl_3COO)_6(THF)_3]$ and $[Fe_2MgO(CHCl_2COO)_6(H_2O)(THF)_2]$; c) essentially different atomic numbers just as coordination environment, $[Fe_2CaO(CCl_3COO)_6(THF)_4]$, $[Fe_2SrO(CCl_3COO)_6(THF)_6] \cdot 2THF$, and $[Fe_2BaO(CCl_3COO)_6(THF)_6] \cdot 2THF$, $[Fe_4Ca_2(\mu_3-O)_2(CHCl_2COO)_{12}(THF)_6]$. The compounds of the last two groups constitute the first examples of *hetero*-trinuclear iron carboxylates containing the non-transition metals. They were used as the suitable precursors in the synthesis of unprecedented (and various -ubрати) tetranuclear 4f-3d clusters assembled *via* carboxylate ligands. In particular, the interaction between $[Fe_2BaO(CCl_3COO)_6(THF)_6] \cdot 2THF$ and $Eu(NO_3)_3$ in acetone solution leads, depending on the temperature, to the formation of the $[Fe_3EuO_2(\mu_3-O)_2(CCl_3COO)_8(THF)_4] \cdot THF$ or $[Fe_3Eu(\mu_3-O)_2(CCl_3COO)_8(THF)_3(H_2O)] \cdot THF$ complexes. Surprisingly, the treating of hexanuclear $[Fe_4Ca_2(\mu_3-O)_2(CHCl_2COO)_{12}(THF)_6]$ compound with neodymium sulfate in water solution yields a mixed-valence $[Fe_3O(CHCl_2COO)_6(H_2O)_3]$ complex characterized by X-ray crystallography.



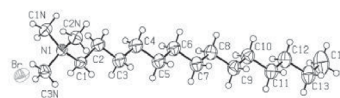
Molecular structure of $[Fe_3EuO_2(CCl_3COO)_8H_2O(THF)_3]$ complex associated with solvate THF molecule.

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s13.m35.p23 **Pseudosymmetry in Tetradecyltrimethylammonium Bromide.** Manuela Ramos Silva, Ana Matos Beja, Jose Antonio Paixao. CEMDRX, FCT, Universidade de Coimbra, 3004-516 Coimbra, Portugal. E-mail: manuela@pollux.fis.uc.pt

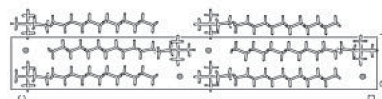
Keywords: Surfactant; Pseudosymmetry; X-ray diffraction

Tetradecyltrimethylammonium bromide is commonly used as a surfactant and germicide. A single crystal grown serendipitously from the residual detergent used to wash laboratory glassware was analyzed showing that the long organic molecules are packed in layers with the tetradecyl chains adopting an extended zigzag form. These long chains are parallel within a layer and antiparallel in alternate layers, featuring a $P2_1/c$ space group. This packing emulates a c-halved unit cell in space-group $P2_1/m$, but this group is not supported by the diffraction data, as many (hkl) reflections were observed with weak but significant intensity having $l = 2n+1$. Refinement in both $P2_1$ and $P2_1/m$ resulted in unrealistic bond lengths and displacement parameters, whereas the inclusion of the weak reflections and refinement in the proper cell revealed the correct structure[1].



The long carbon chain of the cation is not totally planar. Atoms C4 to C14 lie in a plane with a mean deviation of 0.037(3) Å from the least-squares plane. This plane makes an angle of 21.87(3)° with the least-squares plane of the remaining carbons [C1, C2 and C3].

Only a weak intermolecular interaction exists, C1n shares an H-atom with Br with a distance of 3.787(2) Å and an angle of 160.78°.



The conformation of the chain and the hydrogen bond network will be compared to the one found in tetradecyltrimethyl ammonium picrate. The latter compound has 2 independent cations (and anions) in the triclinic cell.

- [1] Ramos Silva *et al.* *Acta Crystallographica* E59 (2003), o1151-o1152.