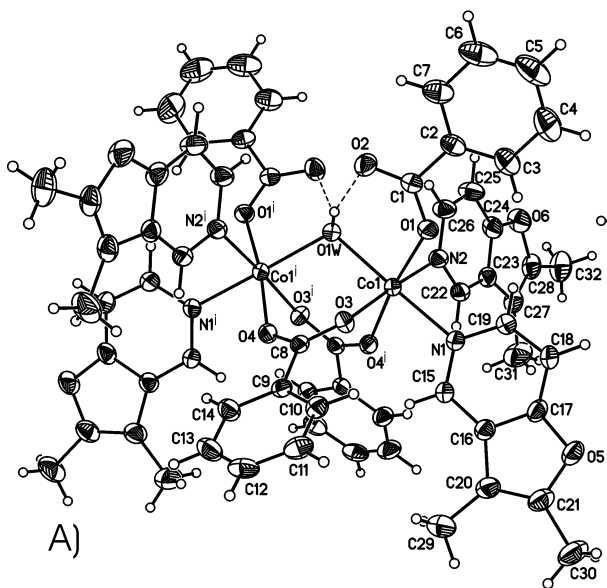


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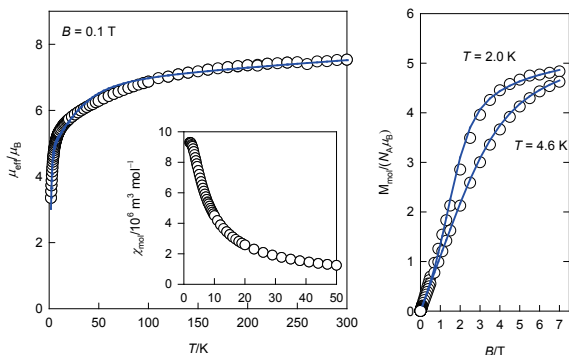
Structure and Magnetism of Dinuclear Cobalt Complexes Containing Furopyridine Derivatives.

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Two dinuclear Co(II) complexes have been prepared and structurally characterized. They resulted from combination of Co(II) benzoate with dimethylfuro[3,2-*c*]pyridine (*Mezfupy*) and/or methylfuro[3,2-*c*]pyridine (*Mefupy*). Both complexes consist of two Co(II) centres bridged by two benzoate and one aqua ligands (Fig. 1): **1** = $[\mu_2\text{-OH}_2(\mu_2\text{-PhCOO})_2\{\text{Co}(\text{PhCOO-}\kappa^1\text{-O})(\text{Mezfupy-}\kappa^1\text{-N})_2\}_2]$ and **2** = $[\mu_2\text{-OH}_2(\mu_2\text{-PhCOO})_2\{\text{Co}(\text{PhCOO-}\kappa^1\text{-O})(\text{Mefupy-}\kappa^1\text{-N})_2\}_2]$. The chromophore consists of the $\{\text{CoOO}'\text{O}'_2\text{N}_2\}$ donor set and the N-donor *Mezfupy* (*Mefupy*) bear function of terminal ligands.



The magnetic data down to 1.9 K confirm a weak antiferromagnetic exchange coupling [1]: $J/hc = -1.05 \text{ cm}^{-1}$, $g_z = 2.18$, $g_x = 2.75$, $D/hc = 36.3 \text{ cm}^{-1}$, $\chi_{\text{TIM}} = 50 \times 10^{-9} \text{ m}^3 \text{ mol}^{-1}$, and $zj = +0.19 \text{ cm}^{-1}$ for **1** (Fig. 2); $J/hc = -1.25 \text{ cm}^{-1}$, $g_z = 2.00$, $g_x = 2.52$, $D/hc = 23.4 \text{ cm}^{-1}$, $\chi_{\text{TIM}} = 50 \times 10^{-9} \text{ m}^3 \text{ mol}^{-1}$, and $zj = +0.17 \text{ cm}^{-1}$ for **2**.



[1] Boča R., Dlhán L., Krutošiková A., Moncol J., *Inorg. Chem.*, submitted.

Keywords: dinuclear Co(II) complexes, structure, magnetism

FA4-MS34-P17

A New Iron(III) Undeca- and Tetradecanuclear Carboxylate Clusters.

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Polynuclear coordination cluster complexes of paramagnetic transition metal ions attract vast attention due to their wide range of magnetic properties, ranging from single-molecule magnetism to spin frustration. The most successful synthetic route to high-nuclearity clusters starts with small metal cages, typically oxo-centered complexes and structure-directing organic ligands that eventually terminate the molecular growth steps. New undeca- and tetradecanuclear Fe(III) pivalate clusters $[\text{Fe}_{11}(\mu_3\text{-O})_7(\mu\text{-OH})_4(\text{O}_2\text{CCMe}_3)_{15}]$ and $[\text{Fe}_{14}(\mu_4\text{-O})_3(\mu_3\text{-O})_9(\text{O}_2\text{CCMe}_3)_{18}(\text{H}_2\text{O})_2]$ have been obtained and characterized by spectroscopy, single-crystal X-ray structure determination, magnetochemical and thermal analysis. In both complexes, flexible pivalate ligands coordinate in 1,3-bridging modes and define the outer surface of the resulting coordination clusters

From a structural perspective, large metal clusters with bridging pivalate ligands are typical examples of molecules with a highly ordered main "heavy" core and statistically/dynamically disordered "light" terminal groups. We here probe if different suggested restraining/constraining models for refinement have significant influence on an ordered part of molecule? How far can we go with "massaging" of objective experimental data? What is "the true point" on this way and what are the limits of structural interpretation for such molecules?

Keywords: molecular magnets, structure refinement, clusters

FA4-MS34-P18

Structure solution of Mesityllithium from powder

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Organolithium compounds are important in research and industrial applications of synthetic chemistry. In fact, only a few structures of aromatic organolithium compounds are known. By reaction of mesitylbromide and *n*-butyllithium in Et_2O at -78°C mesityllithium is obtained as a colourless powder [1]. After indexing of the powder pattern and determination of the space group, the crystal structure of mesityllithium was solved using the simulated annealing algorithm of DASH [2]. The structure investigation was completed by a Rietveld refinement with TOPAS [3]. The compound crystallizes solvent-free due to the strong interactions of lithium with the π -system of the aromatic mesitylene. The short contact from lithium to the aromatic ring leads to zig-zag chains of coordinated lithium atoms.

Structural and chemical details of the title compound will be reported.

[1] Alexander Hübner, Thomas Bernert, Inge Sängner, Edith Alig, Michael Bolte, Lothar Fink, Matthias Wagner, Hans-Wolfram Lerner, *in preparation*. [2] David, W. I. F., Shankland, K., Van de Streek, J., Pidcock, E. & Motherwell, S. (2004). DASH Version 3.0. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England. [3] Coelho, A. (2007). TOPAS-Academic Version 4.1. Coelho Software, Brisbane, Australia.

Keywords: Mesityllithium, powder data, Rietveld refinement

FA4-MS34-P19

Crystal structure of Cu complex with pyridine-2,6-dicarboxylic acid and 9-aminoacridine.

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Recently, we have defined a plan to prepare water soluble proton transfer compounds as novel self-assembled systems that can function as suitable ligands in the synthesis of metal complexes [1,2]. In this regard, we prepared new (AacrH)₂[Cu(pydc)₂] · 3H₂O compound in which (pydcH₂) is pyridine-2,6-dicarboxylic acid and (Aacr) is 9-aminoacridine. Cu^{II} compound crystallized in triclinic crystal system with two molecules per unit cell. The anion was six-coordinate complexes with distorted octahedral geometries around the Cu^{II} centers. The negative charges of [Cu(pydc)₂]²⁻ species in this compound were neutralized with (AacrH)⁺ cations, protonated at the endocyclic nitrogen atom, as counter-ions. Extensive π-π stacking interactions between two aromatic rings of 9-aminoacridine with distances ranging from 3.3498(18) to 3.8718(17) Å, were observed in the title compound. Non-covalent interactions such as hydrogen bonding (consisting O—H...O, N—H...O and C—H...O hydrogen bonds), π-π and C=O...π stacking interactions (with O...π distances ranging from 3.564(2) to 3.834(2) Å) play important roles in stabilizing the structures.

[1] H. Aghabozorg, J. Attar Gharamaleki, M. M. Olmstead and Z. Derikvand, S. Hooshmand, *Acta Cryst.*, 2009, E65, m186. [2] H. Aghabozorg, Z. Derikvand, M. M. Olmstead and J. Attar Gharamaleki, *Acta Cryst.*, 2008, C64, m372.

Keywords: crystal structure, Cu(II) complex, π-π stacking interactions

FA4-MS34-P20

Synthesis, molecular structure, spectroscopic studies of cyanide-bridged Mn(III)Ni(II) Complex.

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The cyanide bridged complex [Mn₂(L1)₂][Ni(CN)₄]₃ (C₂H₆O) 3H₂O (**1**) (L1=(3,5-di tert-butyl-2 hydroxybenzaldehyde-1,2-diaminopropane) has been prepared and characterized by spectroscopic and single crystal X-ray analysis. Single crystal X-ray structure analyses have shown that the crystal structures of **1** is ionic and are built up of [Mn(L1)]²⁺ cations, [Ni(CN)₄]²⁻ anions, water and ethanol molecule. In the complex, two quadridentate ligands are bonded to the Mn(III) ion in a distorted octahedral arrangement and the Ni(CN)₄²⁻ anion remains outside the coordination sphere.

Keywords: Cyano-bridged complex, X-ray diffraction, Schiff Base Ligand

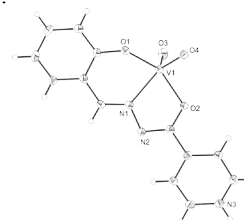
FA4-MS34-P21

Synthesis and crystal structure of a vanadium(V) complex with salicylaldehyde

isonicotinoylhydrazone. Liudmila Gusina^a, Ion Bulhac^a, Diana Dragancea^a, Yurii Simonov^b, Sergiu Shova^b, ^aInstitute of Chemistry, Academy of Sciences of Moldova, Chisinau, Moldova, ^bInstitute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova

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The catalytic properties of vanadium compounds and their effects in biological systems or as therapeutic agents have led to an increasing interest in the coordination chemistry of this element. In this paper we report the synthesis and single-crystal X-ray diffraction study of mononuclear vanadium(V) complex [VO₂(HL)] with salicylaldehyde isonicotinoylhydrazone H₂L. The crystal is monoclinic, space group P2₁/n, *a* = 7.14930(10), *b* = 14.5150(2), *c* = 11.9411(2) Å, β = 94.410(2)°, *V* = 1235.48 Å³, *Z* = 4 for C₁₃H₁₀VN₃O₄. The vanadium(V) atom adopts a square-pyramidal geometry coordinated by the tridentate Schiff base ligand stabilized in *E* form and two oxygen atoms in *cis* positions. The N1–N2 = 1.395(3), N2–C8 = 1.308(3) and C8–O2 = 1.299(3) (Å) bond distances put in evidence the enolate form of the amide functionality. X-ray diffraction study has demonstrated the protonation of the pyridine ring, which was also observed earlier in Fe^{III} and V^V complexes with a related ligand [1,2]. The crystal structure is stabilized by a strong intermolecular N–H...O H-bonds, involving the protonated pyridinic nitrogen and the equatorial oxo ligand (N3–O4', 2.61(2) Å; ∠N3–H...O4' = 164.5°).



[1] Richardson D.R., Bernhardt P.V., *J. Biol. Inorg. Chem.*, 1999, 266. [2] Yu, Q., Li, Ch.-Y., Bian, H.-D., Liang, H., Song, H.-B., Wang, H.-G. *Chinese. J. Struct. Chem.*, 2007, 37.