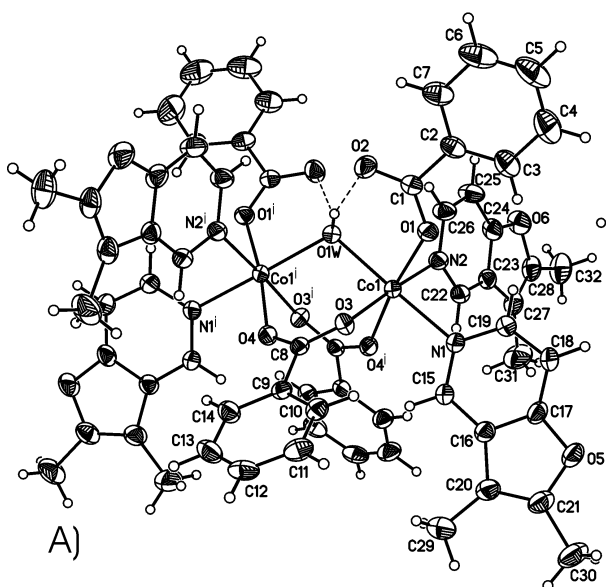


## FA4-MS34-P16

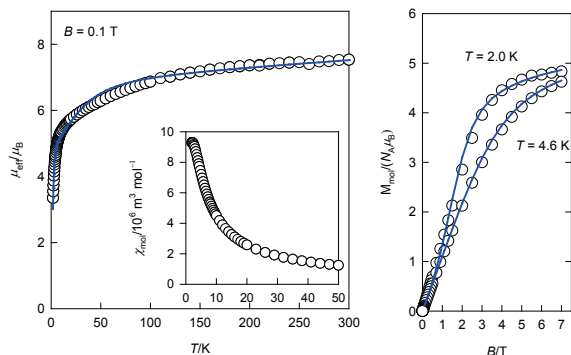
**Structure and Magnetism of Dinuclear Cobalt Complexes Containing Furopyridine Derivatives.**

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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  $\text{Et}_2\text{O}$  at  $-78^\circ\text{C}$  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  $\pi$ -system of the aromatic mesitylene. The short contact from lithium to the aromatic ring leads to zig-zag chains of coordinated lithium atoms.