

DSC/TGA thermal analysis. FT-IR spectra of the compounds indicates the nature of the metal-ligand coordination environment. Presence of  $\nu(\text{O-H})$  shifted to lower energy indicated H-bonded carboxylic acid, while  $\nu_{\text{as}}(\text{COO}^-)$  and  $\nu_{\text{s}}(\text{COO}^-)$  splitting show both monodentate and bidentate carboxylate coordination [2]. Monodentate  $\text{SO}_4^{2-}$  ( $\text{C}_{3v}$ ) and bidentate bridging  $\text{SO}_4^{2-}$  ( $\text{C}_{2v}$ ) modes can also be inferred from infrared spectral analysis.

[1] C. Papatriantafyllopoulou, C.P. Raptopoulou, A. Terzis, J.F. Janssens, E. Manessi-Zoupa, S.P. Perlepes, J.C. Plakatouras, *Polyhedron* **2007**, *26*, 4053-4064. [2] M. Nara, H. Torii, M. Tasumi, *J. Phys. Chem.* **1966**, *100*, 19812-19817.

**Keywords:** metal-picolinate complexes, carboxylic acid, spectroscopy

## MS24.P80

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### Inverse opal-like systems: correlating mesoscale structure and magnetic properties

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A new class of the three-dimensional mesoscale ferromagnetic structure, Inverse Opal-Like Structures (IOLS), is investigated by means of microradian X-ray Diffraction (XRD) and polarized Small-Angle Neutron Scattering (SANS). The samples are synthesized by filling the voids of artificial opals with cobalt or nickel precursors and subsequent removing the initial template in order to leave three-dimensionally ordered porous films consisting of quasi-tetrahedra and quasi-cubes which are connected by vertices.

The microradian XRD reveals the type and degree of imperfection of opal-like structures. It was shown that the inverse OLS ordered in the twin FCC structures with the lattice constant of  $640 \pm 10$  nm but also with clear tendency to the random hexagonal close-packed (RHCP) structure along the [111] axis.

The magnetic properties of IOLS were studied by polarized SANS technique with the analysis of the magnetic contribution and nuclear-magnetic interference of the diffraction peaks. The complex magnetic structure appears upon application of the magnetic field with non-homogeneous distribution of magnetization density. Such distribution is determined by the combined effect of the easy-plane geometry of the film and the principal axes of the opal-like structure with respect to the applied field direction.

**Keywords:** opal-1, magnetism-2, SANS-3

## MS24.P81

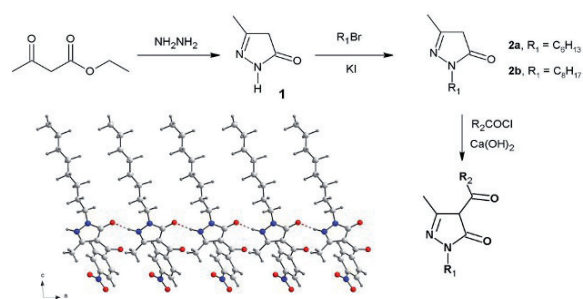
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### A supramolecular approach to the analysis of the crystal structures of some 1-Alkyl-3-methyl-4-acyl-5-pyrazolone derivatives

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For theoretical and practical reason pyrazolones are an important group of nitrogen heterocyclic organic compounds. They find applications as analgesic and anti-inflammatory drugs, dyes, chelating extractants for numerous metal ions [1]. Pyrazolones have also attracted much attention because they exhibit prototropic tautomerism and they have been extensively studied both in solution and in the crystalline phase. Pyrazolones have also been studied as photochromic and luminescent materials. Coordination chemistry of pyrazolones is also very important; consequently considerable effort has been devoted to have a better knowledge of both ligands and metal complexes based on pyrazolone derivatives.

Most 3-methyl-4-acyl-pyrazolones reported to date are 1-aryl derivatives, in some few cases it is possible to found 1-alkyl examples like methyl or t-butyl, but the 1-n-alkyl-pyrazolones are scarce. On the other side, it was shown that 5-pyrazolone can be easily alkylated at N-1 with primary alkyl halides yields being very good [2]. Alkylpyrazolones underwent electrophilic substitution at C-4 the same way 1-arylpyrazolones do. Thus, 1-n-alkylpyrazolones can be acylated following the procedure reported by Jensen [3]. The 1-aryl-4-acylpyrazolones are isoelectronic with  $\beta$ -diketones and their coordination chemistry is very well known. The coordination chemistry and tautomeric behaviour of some 1-n-alkyl-4-acylpyrazolones is even less known. In this presentation the synthesis and crystallographic data of 1-alkyl-3-methyl-4-acyl-5-pyrazolones and their Cu(II) complexes are discussed.



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[1] F. Marchetti, C. Pettinari, C. Pettinari, *Coord. Chem. Rev.* **2005**, *249*, 2909. [2] J. Belmar, J. Alderete, M. Parra, C. Zúñiga, *Bol. Soc. Chil. Quím.* **1999**, *44*, 367. [3] B.S. Jensen, *Acta. Chem. Scand.* **1959**, *13*, 1668.

**Keywords:** crystal engineering, acylpyrazolones, Cu-complexes

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### Amide to amide interactions: from strong to weak hydrogen bonds in bis-(quinoxaline-carboxamide) functionality

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Deliberate design of molecules to build supramolecules in crystals with particular properties has become a very attractive area of research. A productive strategy in crystal engineering is to consider the molecules with functional groups that form robust synthons [1]. Crystal packing is the result of the optimization of various possible intermolecular interactions between the molecules. Structures including carboxylic