derivatives seem to be good candidates to obtain new materials because of the versatile behaviour of this metal[2]. For this reason, our research has been focused in the synthesis and characterization of hybrid vanadates with aromatic and aliphatic amines[3]. In this work we present the comparative study of a hybrid vanadate, $Co(pym)(VO_3)_2$ (pym=pyrimidine) and an inorganic one $Co(H_2O)_2(VO_3)_2.2H_2O$ with closely related structures.

The three-dimensional $Co(pym)(VO_3)_2$, **1**, has been synthesized under mild hydrothermal conditions. The crystal structure of **1** was solved using single-crystal X-ray diffraction data, taking into account that the crystals are twins of two components. Compound **1** crystallizes in the monoclinic system, space group C2/c, a= 12.899(5) Å, b= 9.899(2) Å, c= 7.051(1) Å, β= 111.41(3) º, Z= 4. The crystal structure is built up from edge sharing $VO_5$ trigonal bipiramid double chains and $[CoO_4pym]_n$ chains. This resembles to the structure of the $Co(H_2O)_2(VO_3)_2.2H_2O$ compound[4], **2**. For this reason a comparative study of their properties was carried out.

Magnetic measurements of **1** reveal the existence of a ferromagnetic transition. This fact was confirmed with magnetization measurements. The ferromagnetic transition was also studied by specific heat measurements. However, **2** shows an antiferromagnetic behaviour with a metamagnetic transition at low temperature. The comparative study of the magneto-structural correlations reveals that the magnetic interactions in **1** are propagated via pyrimidine molecules, while in **2** the unique magnetic exchange pathway is the one extended by the vanadate groups.

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**Keywords: Organic inorganic hybrid materials, Magnetic properties, Structure-magnetism relationships.**

## FA4-MS33-P04

### Magneto-Structural D-Correlations in Metal Complexes.

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Determination of the molecular and crystal structure by X-ray diffraction is an important step in the course of the characterization of new molecule-based magnetic materials. In addition to determination of molecular geometry, in some cases a detail analysis of the structural properties can give relevant information on different magnetic phenomena itself. For example, the correlation of the isotropic exchange coupling constant *J* with the bridging angle in dinuclear complexes is well-known [1]. However, the relationship between structural properties and single-ion magnetic anisotropy of metal complexes is also of a great interest. Nevertheless, such correlation has not yet been clearly formulated.

Unlike magneto-structural J-correlations, our new magneto-structural D-correlation interrelates the zero-field splitting parameter *D* withdrawn from the magnetic data with the structural tetragonality $D_{str}$. The possibility of correlating these parameters has been outlined gradually [2, 3].

The correlation allows to predict that negative zero-field splitting occurs for the tetragonally compressed nickel(II) complexes. Cobalt(II) complexes in octahedral ligand-field have high-spin ground state with a distinct spatial symmetry and thus such a correlation shows a substantially different structure-magnetism relationship. Mn(II)/(III) complexes and systems with angularly distorted chromophores have been also investigated.

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**Keywords: metal complexes, magnetic anisotropy, magneto-structural correlations**

## FA4-MS33-P05

### The structure of poly[di-$\mu_3$-acesulfamato-O,O:O';O':,O,O-di-$\mu$-acesulfamato-O,O;N-di-$\mu$-aqua-dicalcium(II)]: a two dimensional coordination polymer.

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The crystal structure of the title compound, $C_{32}H_{40}Ca_4N_8O_{36}S_2$, determinated at 293 K. The structure contains Alkali Earth Metal, Ca, and acesulfam ring. The crystal that is two dimension coordination polymer contain three intramolecular hydrogen bonds, but no signification intermolecular hydrogen bonds. The structure consists of sheets in the bc plane. The crystal structure with acesulfam ring and Ca ion is first polymeric structure.

**Keywords: Alkali Earth Metal, Acesulfam**

## FA4-MS33-P06

### Non-triglyceride structuring of edible oils and emulsions.

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The structure of oil-continuous products, such as margarine or butter, is based on a network of small crystallites of triglycerides (also known as triacylglycerols or TAGs). Low molecular weight structuring agents that can serve as an alternative to crystallising triglycerides in edible oils have raised considerable interest in recent years. The requirement that potential structurants should at least hold the promise to be allowed in food applications is a severe limitation. Nevertheless, several systems have been identified [1], amongst which the class of γ-oryzanol + sterol organogelators is the most intriguing representative [2].

Mixtures of γ-oryzanol and β-sitosterol can form transparent organogels in edible oils. This process is a nice example of molecular self-assembly, where γ-oryzanol and β-sitosterol molecules form very well-defined supramolecular entities.
Small-angle X-ray scattering (SAXS) was used to elucidate the microstructure of the building blocks of these organogels in sunflower oil [3]. The measurements were performed at the high-brilliance ID2 beamline of the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, allowing collection of SAXS data in the range $0.06<q/nm-1<4.5$. Differential Scanning Calorimetry (DSC) was used to study the dissolution, melting and crystallisation behaviour of these systems during a heating-cooling-heating cycle.
It was found that the γ-oryzanol + β-sitosterol system forms tubules with a diameter of 7.2±0.1 nm and a wall thickness of 0.8±0.2 nm. Tubules prepared with γ-oryzanol-rich structurant show the least bundle formation, and can be supercooled during formation most easily. The tubes vanish at the melting point of the gel, in agreement with the loss of structuring capacity as observed in earlier experiments.
Moreover, a number of alternative sterols (e.g. stigmasterol, cholesterol, cholestanol) can replace β-sitosterol in the tubules. The diameter of the tubules for these systems varies between 7.2 and 8.0 nm, the wall thickness between 0.6 and 1.1 nm. The microstructure of the sterol(esters) in emulsions differs from that in pure oil.

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**Keywords: organogels, self-assembly, small-angle X-ray scattering**

## FA4-MS33-P07

### Synthesis and Structural Resolution of C14H13N3S·H2O, a new Thiosemicarbazone.

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Thiosemicarbazones, a class of compounds possessing a wide spectrum of potential medicinal applications, have been studied for their antitumoral, antiviral, antibacterial, antimalarial, antifungal, anti-inflammatory and anti-HIV activities [1]. These properties are thought to arise from the metal-chelating ability of these ligands. In almost all cases, the ligands are bidentate and bind to the metal through the S and hydrazinic N atoms, although there are examples of them acting as monodentate ligands binding only through sulphur [2]. The synthesis, crystal structure and electron density topological properties for title compound C14H13N3S·H2O are reported here.
The thiosemicarbazone adopts an E conformation with a trans configuration observed about the C=N bond. The dihedral angle between benzene ring and the thiosemicarbazone moiety is 4.67(1)°, this value suggests that are nearly coplanar, due to the delocalized π-electrons in the benzaldehyde thiosemicarbazone fragment.
The water molecules are involved in an extensive intermolecular N—H···O hydrogen bonds and O—H···S interactions, which link the molecules into chains extended along b axis. Sulphur atom is also involved in N—H···S intermolecular interactions, favouring the crystal packing in the ac plane. An intramolecular N—H···N hydrogen bond contributes to stabilize the molecular conformation. The intermolecular distance value between centroids of the planar rings in the b axis direction (6.350 Å), does not suggests π-stacking interactions between parallel molecules.

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**Keywords: Thiosemicarbazones, Synthesis, Structural Determination, Electron Density Topology**

## FA4-MS33-P08

### Structural and systematic studies of a 3x3 isomer grid of nine *N*-(fluorophenyl)-pyridinecarboxamides

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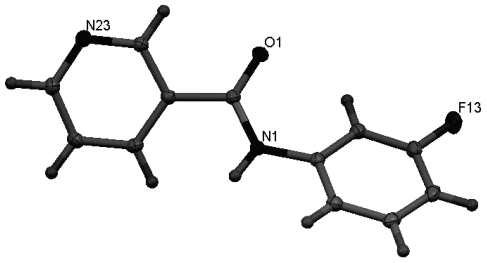
Nine **NxxF** isomers (**x** = 4-, 3- or 2-**N**/**F** substitution) were investigated and compared to determine factors underpinning (*a*) the roles of the **F**/**N** atom substituents on molecular conformation and overall supramolecular aggregation, (*b*) competition between intermolecular amide…amide (in **NppF**) or intra-/intermolecular amide…pyridine hydrogen bond formation and (*c*) general structural and physico-chemical properties and trends.




Crystal structure analyses of the nine **NxxF** isomers reveal different primary interactions as N-H…N or N-H...O=C. **NpmF** and **NpoF** are isomorphous and the latter is also disordered. Conformational analysis of the **NxxF** molecular conformations from DFT calculations differ from the crystal structure results for several isomers and highlighting the co-operative effects of intra-/intermolecular interactions in the solid state.