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Keywords: anils, cyclodextrin, molecular imprint

MS24.P77

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Supramolecular study of μ-oxo iron(III) porphyrin malaria pigment model compounds

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Malaria is an infectious disease caused by the parasite *Plasmodium falciparum* invading red blood cells. Toxic free heme released by the parasitic destruction of hemoglobin is detoxified by conversion to malaria pigment. The μ-oxo TPP and OEP heme complexes have been studied as malaria pigment model systems [1]. The current study focuses on structure correlation of these and $[Fe(PPIX)]_2(\mu\text{-}O)$ in an effort to better understand the relationship between the spectra of malaria pigment and the μ-oxo heme complexes. The supramolecular interactions between propionate chains, C−H···O and interplanar interactions, C−H···π in $[Fe(PPIX^*)]_2(\mu\text{-}O)$ are observed. The tight H···O interaction distances are 2.62(4) Å while the H···π distances are 2.84(5)-2.93(5) Å.

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Keywords: structure modeling, supramolecular structure, malaria pigment models

MS24.P78

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Crystal structures of a series of bisazomethine dyes derived from 4-(Dimethylamino)-2-alkoxybenzaldehydes

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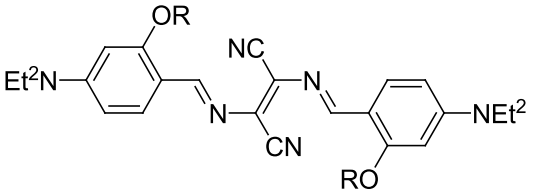
Bisazomethine dyes derived from diaminomaleonitrile with aminobenzaldehydes are known as a potential dye forming J-aggregates in a solid state like vapour-deposited films [1-3]. We have synthesized a series of bisazomethine dyes based on alkoxy-substituted aminobenzaldehydes shown in the figure in order to investigate the effect of alkoxy-substitution (OR) of the phenyl rings in vapour-deposited films [4]. Here we report crystal structures of the eight bisazomethine dyes focusing on the effect of the substitution on their molecular arrangement in a crystalline state.

All the dyes were found to have their molecules π–π stacked in the two-dimensional (D) staircase molecular arrangements. Within the staircase stacking layer, molecules are stacked along the long molecular axis with smaller slip angles than the critical angle of dipole-dipole interactions. This 2-D stacking layer is aligned along the short molecular axis to form 3-D crystal structure with spacing related to the length of the substituent R. The effect of R on their molecular arrangement in a crystalline state showed that the interlayer distance between adjacent 2-D stacking layers changed from 8.51 Å to 14.52 Å, when the length of the substituent is less than C10. These structural characteristics were interpreted by lattice energy calculations on the basis of the intermolecular interactions and crystal energies. The first and second energetic contributions to the lattice energy were given from a stacking molecular pair characterized by a large slip angle. In addition, stacking pairs having small slip angles were the third and fourth contributors. In **8**, however, the molecules are no longer stacked in the same manner as in the other dyes in which the specific molecular pair between their long alkyl chains of the alkoxy substituents gave the third and fourth energetic contributions.

In this dye system, the substituents on the phenyl rings can be used as practical parameters for spatial control between the 2-D stacking layers without significant changes in the stacking layer itself, when the length of R is less than C10.



1 R = $C_6H_5CH_2$, **2** R = C_6H_5, **3** R = C_2H_5, **4** R = C_3H_7, **5** R = C_5H_{11}, **6** R = C_7H_{15}, **7** R = C_8H_{17}, **8** R = $C_{10}H_{21}$

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Keywords: crystal_engineering, organic_dye, molecular_aggregate

MS24.P79

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Crystallization of mixed ligand complexes of $M(SO_4)$ with picolinic acid and carboxylic acids (M = Mn, Zn)

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A variety of related metal complexes can be prepared from multifunctional ligands which are capable of monodentate and bidentate coordination. The ligands used in this study can also bridge metal atoms or form chelate rings leading to synthesis of new metal-picolinate-carboxylate compounds utilizing the several metal-picolinate binding modes [1]. The mixed ligand complexes prepared from M(II) sulfate (M = Mn, Zn) reacted sequentially with picolinic acid as a primary ligand (L1) and carboxylic acids (salicylic acid, phthalic acid and succinic acid) as a secondary ligand (L2). XRD of the crystalline products obtained from room temperature reaction of 1:1:1 (M:L1:L2) mole ratio showed that new compounds were formed. Composition of the crystals was characterized by elemental analysis, SEM/EDS microscopy, and

DSC/TGA thermal analysis. FT-IR spectra of the compounds indicates the nature of the metal-ligand coordination environment. Presence of ν(O-H) shifted to lower energy indicated H-bonded carboxylic acid, while $\nu_{as}(COO^{-})$ and $\nu_{s}(COO^{-})$ splitting show both monodentate and bidentate carboxylate coordination [2]. Monodentate SO_4^{2-} (C_{3v}) and bidentate bridging SO_4^{2-} (C_{2v}) modes can also be inferred from infrared spectral analysis.

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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 ± 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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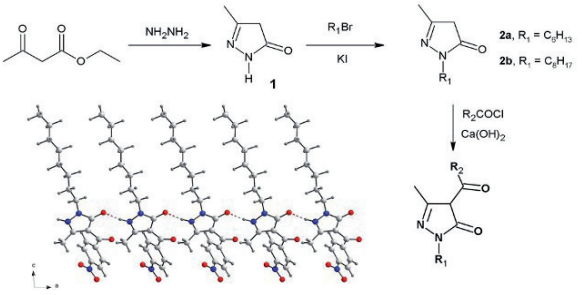
For theoretical and practical reason pyrazolones are an important group of nitrogen heterocyclic organic compounds. They find applications as analgesic and anti-inflammatory drugs, dyes, chelating extractants for numerous metal ions [1]. Pyrazolones have also attracted much attention because they exhibit 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-pirazolones 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 β-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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Keywords:crystal engineering, acylpyrazolones, Cu-complexes

MS24.P82

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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