Mavridis, *J Photochem. Photobiol. A: Chem*. **2011**, *217*, 293–298. [2] T. Aree, N. Chaichit, *Carbohydr. Res*. **2008**, *343*, 2285-2291.

Keywords: anils, cyclodextrin, molecular imprint

MS24.P77

Acta Cryst. (2011) A**67,** C387

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.

[1] R. Puntharod, G. T. Webster, M. Asghari-Khiavi, K. R. Bambery, F. Safinejad, S. Rivadehi, S. J. Langford, K. J. Haller, B. R. Wood, *J. Phys. Chem. B* **2010** *114(37)* 12104-12115

Keywords: structure modeling, supramolecular structure, malaria pigment models

MS24.P78

Acta Cryst. (2011) A**67,** C387

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

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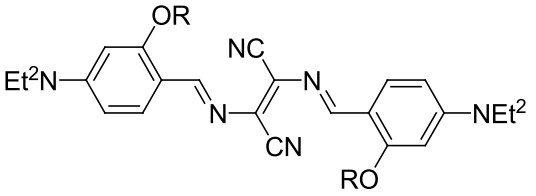
Bisazomethine dyes derived from diaminomaleonitrile with aminobenzaldehydes are known as a potential dye forming J-aggregates in a solid state like vapour-deposited films [1-3]. We have synthesized a series of bisazomethine dyes based on alkoxy-substituted aminobenzaldehydes shown in the figure in order 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 = $C_{10}H_{21}$

[1] K. Shirai, M. Matsuoka, K. Fukunishi, *Dyes and Pigments* **2000**, *47*, 107-115. [2] S. Matsumoto, T. Kobayashi, T. Aoyama, T. Wada, *Chemical Communications* **2003**, *15*, 1910-1911. [3] S. Matsumoto, K. Shirai, K. Kobayashi, T. Wada, M. Shiro, *Zeitschrif für Kristallographie* **2004**, *219*, 239-243. [4] B. S. Kim, D. Kashibuchi, Y. A. Son, S. H. Kim, S. Matsumoto, *Dyes and Pigments* **2011**, *90*, 56-64.

Keywords: crystal_engineering, organic_dye, molecular_aggregate

MS24.P79

Acta Cryst. (2011) A**67,** C387-C388

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