

β -cyclodextrins make a dimer facing bigger rims to each other. Inside the dimer, two l-menthols are included with their molecular axes in the same direction.

Keywords: inclusion complex, β -cyclodextrin, l-menthol

MS38.P05

Acta Cryst. (2011) A67, C487

Self-assembly of metal trischelates to afford extended structures for porous applications

Tia Jacobs, Michael J. Hardie, School of Chemistry, University of Leeds, Leeds, (United Kingdom). E-mail: t.jacobs@leeds.ac.uk

The search for porous materials and design principles to achieve this aim is ever increasing. These materials have a variety of potential applications such as catalysis, gas separation and storage. Problems that exist in the assembly of porous materials are the tendency of molecules to pack closely in the solid state, thereby obliterating free space. In recent years the use of polymeric metal-coordination compounds for porous applications has increased with the realisation that judicious choice of metal centre and rigid bridging ligand can afford two- and three-dimensional solids that feature the desired characteristics [1, 2, 3]

Work will be presented where octahedral trischelate complexes based on functionalised 2,2'-bipyridine ligands are linked into two- and three-dimensional networks using a variety of supramolecular interactions. The stability of these crystalline materials toward evacuation and solvent-loss will be shown, as well as their permeability to gasses as proven by gas sorption.

[1] S.R. Batten, R. Robson, *Angew. Chem. Int. Ed.* **1998**, *37*, 1461-1494. [2] B. Moulton, M.J. Zaworotko, *Chem. Rev.* **2001**, *101*, 1629-1658. [3] S.L. James, *Chem. Soc. Rev.* **2003**, *32*, 276-288.

Keywords: self-assembly, supramolecular, bipyridine

MS38.P06

Acta Cryst. (2011) A67, C487

Novel coordination polymers based on rigid and flexible organic ligands and Cu(II) ions

Ana Belén Lago, Rosa Carballo, Emilia Garcia-Martínez, Sabina Rodríguez-Hermida, Ezequiel M. Vázquez-López. Departamento de Química Inorgánica, Facultad de Química, Edificio de Ciencias Experimentales, Universidad de Vigo. E-36310 Vigo, Galicia. (Spain). E-mail: ablago@uvigo.es

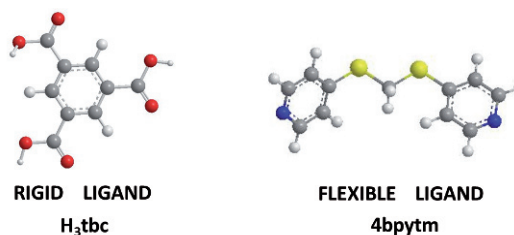
Dynamic polymers based on monomeric components connected through either labile noncovalent interactions or reversible covalent bonds, are the subject of intense investigation. [1] A special class is formed by coordination polymers, where the control of the polymerization is made through metal-ion coordination bonds. In addition, the presence of noncovalent interactions along the polymeric backbone results in that the material could exhibit reversible polymerization/depolymerization properties. [2] Many of the architectures reported to date are based upon rigid linear linker ligands, with less efforts focusing on the use of ligands showing conformational flexibility. The use of flexible ligands can lead to the formation of interesting architectures without loss of control in the self-assembly process.

We have performed an investigation on the formation of copper(II) coordination compounds based on the use of the 1,3,5-benzenetricarboxylic acid (H_3btc) and the spacer with conformational

flexibility, bis(4-pyridylthio)methane (4bpytm). As result of this study two new coordination polymers are prepared and characterized: $^1_\infty[Cu(H_2btc)_2(4bpytm)]$ (**1**) and $^2_\infty[Cu(Hbtc)(4bpytm)_2] \cdot H_2O$ (**2**). Both compounds are obtained as a mixture by a solvothermal procedure. The optimization of the synthetic route allowed the isolation of the pure phases in a high yield.

The 1D covalent network (**1**) is achieved by the bridging role of 4bpytm ligand between the copper(II) ions, with the biprotonated H_2btc^- ligand acting as terminal ligand. 4bpytm produce also chains in (**2**) that are further pillered by the monoprotinated ligand $Hbtc^-$ to form high robust layers. An interesting feature is that in both compounds exist different open sites per copper atom that form coordinatively unsaturated metal centres (UMCs) that can strongly interact with guest molecules. The use of a ligand with carboxylate groups partially protonated makes that the corresponding supramolecular associations are organized by the effect of different OH...O hydrogen bonds.

Acknowledgments: A.B.L. thanks to Xunta de Galicia for a postdoctoral-fellowship "Ángeles Alvariño". Financial support from Xunta de Galicia (Spain) (research project 10TMT314002PR) is gratefully acknowledged.



[1] C.F. Chow, S. Fujii, J.M. Lehn. *Angewandte Chemie* **2007**, *46*, 5007-5010.

[2] J.B. Beck, J.M. Ineman, S.J. Rowan. *Macromolecules* **2005**, *38*, 5060-5068.

Keywords: copper complexes, crystal structures, metallosupramolecular chemistry.

MS39.P01

Acta Cryst. (2011) A67, C487-C488

Structural studies and electron density analysis of thiophene based compounds

Maqsood Ahmed,^a Sajida Noureen,^b Philippe C. Gros,^b Benoit Guillot,^a Christian Jelsch,^a Claude Lecomte,^a ^aUMR CNRS 7036(CRM²), Laboratoire de Cristallographie, Résonance Magnétique et Modélisation, ^bUMR CNRS 7565 (SOR), Synthèse Organométallique et Réactivité, Faculté des Sciences et Technologies - UHP, BP 239, 54506 Vandœuvre-lès-Nancy cedex, (France). E-mail: maqsood.ahmed@crm2.uhp-nancy.fr

As the galloping energy demands of the world combined with the environmental concerns call for looking alternate and cleaner sources of energy, much attention is being diverted to the renewable sources of energy, including the solar energy. Dye sensitized solar cells (DSSCs) are proving to be a potential alternate for the conventionally used semiconductor based solar cells [1]. They offer many advantages such as tuneable electronic properties, especially the band gap, by chemical modifications and substitutions. In this context, thiophenes and their substituted homologues have attracted much attention of the scientific community as the starting materials for the synthesis of organic dyes and metal organic complexes worth applicable in DSSCs. It is considered that the backbone retains its π -conjugated coplanar conformation if the long alkyl chain is substituted at a suitable