

coefficients as determined from variable temperature x-ray diffraction. Molecular dynamics is used to fully characterise ligand movement, and understand the extend to which framework flexibility determines mechanical behaviour.

[1] A.K. Cheetham, C.N.R. Rao, *Science*, **2007**, *318*, 58-59. [2] N. Lock *et al.*, *J. Phys. Chem. C* **2010**, *114*, 16181-16186. [3] T. D. Bennett *et al.*, *Angew. Chem. Int. Ed.* **2011**, *50*, 1-6.

Keywords: metal-organic frameworks, flexibility, molecular dynamics

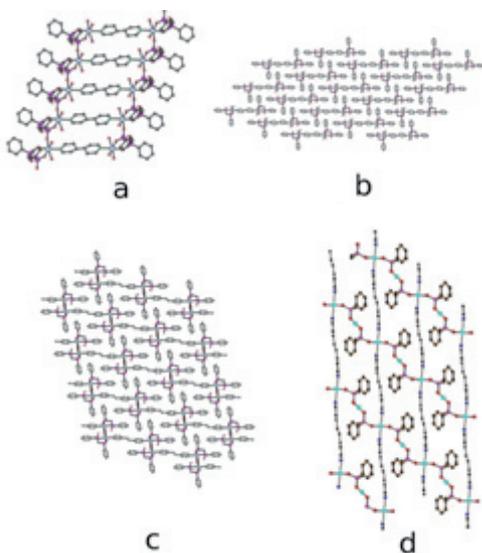
MS38.P03

Acta Cryst. (2011) **A67**, C486

Polymer dimensionality lead by supramolecular interactions in cobalt system

Annalisa Guerri,^a Ferdinando Costantino,^b Andrea Ienco,^c Stefano Midollini,^c ^aDepartment of Chemistry, University of Florence (Italy), ^bDepartment of Chemistry, University of Perugia (Italy), ^cCNR-ICCOM, (Italy). E-mail: annalisa.guerri@unifi.it

Supramolecular forces are involved in the building of the three-dimensional structure in the solid state [1]. Few years ago, it has shown that in metal inorganic organic hybrids the metal coordination environment can be forced by non-covalent interactions. The close packing of 2,2'-bipyridine ligands was responsible for the uncommon trigonal prismatic coordination of Mn(II). The normal octahedral Mn(II) coordination was restored when the intercalation of the bipyridine was prevented using substituted bipyridines [2].



We report here a series of hybrid inorganic organic polymers $[Co(pcp)(4,4'-bipy)_{0.5}2H_2O]_n$ (**1**), $[Co(pcp)(bpye)_{0.5}H_2O]_n$ (**2**), $[Co(pcp)(bpyet)_{0.5}H_2O]_n$ (**3**) and $[Co(pcp)(bpyet)_{0.5}]_n$ (**4**) where pcp = P,P'-diphenyl-methylene-diphosphinato, 4,4'-bipy = 4,4'-bipyridine, bpye = 1,2-bis(4-pyridyl)ethane, bpyet = 1,2-bis(4-pyridyl)ethene).

In Figure 1 are shown 1D ribbon in **1** (a) and the packing view of **1** (b) and of **2** (c) parallel to the ribbon, finally the packing view of **4** (d).

In the 1D polymer of **1**, the ribbons of $[Co_2(pcp)_2bipy]$ are connected by hydrogen bonds (Figure 1a and 1b) while **2** and **3** are built by 2D plane formed by the same kind of 1D ribbons that are covalent bonded by water molecules. The view of the packing parallel to the ribbons shows the same type of arrangement of the phenyl rings

of pcp and of the bi-pyridines. For **4**, a totally different 2D network was found with 1D columns of $[Co(bpyet)]$ connected by square planar $Co(pcp)_2$ units (Figure 1d). The role of the bipyridine and its length in the formation of the network will be discussed.

[1] J.M. Lehn *Supramolecular Chemistry* **1995** Wiley. [2] A. Grirrane, A. Pastor, A. Galindo, D. del Rio, A. Orlandini, C. Mealli, A. Ienco, A. Caneschi, J. Fernandez Sanz *Angew. Chem. Int. Ed.*, **2005**, *44*, 3429.

Keywords: metallorganic polymers, diphosphinate, supramolecular chemistry

MS38.P04

Acta Cryst. (2011) **A67**, C486-C487

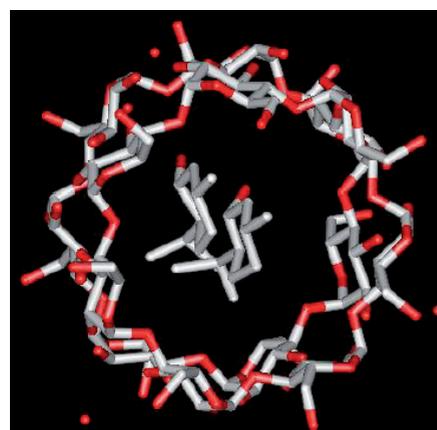
Inclusion Complex of β -Cyclodextrin and l-Menthol

Yasushi Kai,^a Masaki Yamamoto,^a Nobuko Kanehisa,^b Tsuyoshi Inoue^b ^aDepartment of Environmental and Biological Chemistry, Fukui University of Technology, Fukui. ^bDepartment of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, (Japan). E-mail: kai@fukui-ut.ac.jp

Cyclodextrins are the cyclic oligosaccharides composed of the glucopyranoses linked by α -1,4-glucoside bond. There are three common cyclodextrins with 6, 7 or 8 D-glucopyranosyl residues, α -, β - and γ -cyclodextrin respectively. Cyclodextrin has the truncated corn shape with hydrophilic OH substituents outside and hydrophobic cavity inside the molecule. The secondary alcohols (2-OH and 3-OH) make bigger and primary alcohols (6-OH) make smaller rims of truncated corn structure. Therefore, cyclodextrin can include the water insoluble molecules inside its cavity. This property is applied for various reagents to solubilize in water, stabilize from oxidation, recognize a molecule, or transfer a drug. Menthol has local anesthetic and counterirritant qualities, and it is widely used to relieve minor throat irritation. Menthol is included in many products such as toothpaste, chewing gum, cigarette etc. To keep the function of menthol, cyclodextrins are often included in these products. In order to understand the molecular function of cyclodextrin in these products, the crystal structure of β -cyclodextrin and l-menthol was determined by the X-ray diffraction method.

The inclusion complex of β -cyclodextrin and l-menthol crystallized in monoclinic space group $P2_1$ with cell parameters of $a=15.2487(7)$, $b=32.487(1)$, $c=15.3835(5)\text{\AA}$, $\beta=101.712(1)^\circ$, $V=7462.2(5)\text{\AA}^3$, $Z=2$, $F.W.=2582.52$. Two β -cyclodextrins and two l-menthols are in the asymmetric unit. The X-ray diffraction data were collected on Rigaku RAPID diffractometer. The crystals include many crystalline waters and were very unstable in air. Thus, the data measurements were carried out at -150 deg. using flash cooling method. In total, 33,583 independent reflections were observed ($R_{int}=0.0293$). Crystal structure was solved by direct method (SHELXD) and refined by full-matrix least-squares on F^2 (SHELXL-97). The present $R1$ is 0.1100.

The crystal structure is shown in the figure. Two



The detailed molecular interactions between β -cyclodextrin and l-menthol will be discussed.