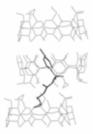


The asymmetric unit contains two  $\beta$ CD molecules and two guest molecules statistically disordered over 2 positions with s.o.f. of 0.5. The stacking of the two host molecules along the c-axis generates dimers held together by seven H-bonds via the secondary hydroxyl groups. The geometries of the two guest molecules and their interactions are very similar. The 2,4-dichlorophenyl moiety of the guest is inside the  $\beta$ CD cavity, whereas the 5-chlorophenol expands in the space between the primary sides of two host molecules. The dihedral angle between the two phenyl rings is 81°. Tolbutamide, 1-butyl-3-(*p*tolysulfonyl)urea (TBM), is an oral hypoglycemic agent insoluble in water. Complexation of TBM with  $\beta$ CD improves its dissolution rate and solubility, which is believed to be the rate-determining step for its absorption from the gastrointestinal tract.



The inclusion complex of  $\beta$ CD/TBM was crystallized and data were collected at room temperature (monoclinic, C2 with a= 19.225Å, b= 24.547Å, c= 15.708Å,  $\beta$ = 109.652°). The structure has been refined up to  $R_1 = 0.1054$ . Two  $\beta$ CD molecules, related by the 2-fold axis and held together by seven H-bonds via the secondary hydroxyl groups, form also dimers, in the cavity of which a TBM molecule is encapsulated. The aromatic ring of the guest is located in the secondary side of the CD and the chain sticks out between the primary sides of two hosts. The N-atoms of the urea group H-bond to hydroxylic groups of the latter pointing inside. The 2-fold axis of the lattice generates a  $\beta$ CD dimer. However, one guest molecule occupies the dimer cavity in a statistical way (the host: guest ratio is 2:1). The dimers align head-to-head along the c-axis forming infinite channels. Channel formation is strengthened by H-bonds between primary hydroxyl groups existing in a variety of orientations.

## **MS18 P07**

Synthesis, characterisation and X-ray study of cobalt (II) complex: [Dimalonato tetraaqua cobalt (II)]  $[Co(C_4H_3O_4)_2(H_2O)_4]$  Jawher Abdelhak, Sawssen Namouchi Cherni, Mohamed Faouzi Zid & Ahmed Driss Laboratoire de Matériaux et Cristallochimie, Département de chimie, Faculté des Sciences, 2092 El Manar, Tunis, Tunisia. E-Mail: jawherabd@hotmail.com

## Keywords: cobalt compounds, characterization method, magnetic crystal structures.

The investigations of novel complexes represent an intense interest of chemical research; this is driven to a large extent by their interesting properties and their potential practical applications [1-3]. In addition, mixed ligand-metal complexes of some organic oxygen-donors ligands continue to attract attention because they play an important role in biological systems [4].

The title compound was synthesized by slow evaporation of solution at room temperature it has been characterized by X–ray diffraction, IR spectral analysis and UV–vis spectroscopy. The natural elements are detected by the EDX on a scanning electron microscope. The thermal analysis shows that the dehydration of the compound occurs in agreement with the structural features. The temperature dependence of the molar magnetic susceptibility,  $\chi_M$ , was measured on a polycristalline sample in the temperature range 5-300 K using a SQUID magnetometer.

The structure was determined by X-ray diffraction on single crystal. This salt crystallizes in the triclinic space group *P*-1 with a = 5.241(1) Å, b = 7.362(1) Å, c = 9.268(1) Å,  $\alpha = 109.15(2)^{\circ}$ ,  $\beta = 104.39(3)^{\circ}$ ,  $\gamma = 93.15(1)^{\circ}$ , V = 323.6(3)Å<sup>3</sup> and Z= 2. Crystal structure has been determined and refined to R = 0.021 and wR = 0.057.

The framework structure of  $[Co(C_4H_3O_4)_2(H_2O)_4]$  is consisted by  $Co^{II}$  ions laying in inversion centers and are six fold coordinated by oxygen atoms from two malonate anions and four water molecules to form a slightly distorted octahedron. The H atoms form hydrogen bonds to neighboring O ensure the cohesion and stability of the molecular packing.

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## **MS18 P08**

Solvent induced transformations in a supramolecular organic zeolite <u>Michela Brunelli</u><sup>a</sup>, Consiglia Tedesco<sup>b</sup>, Loredana Erra<sup>b</sup>, Ivano Immediata<sup>b</sup>, Valeria Cipolletti<sup>b</sup>, Carmine Gaeta<sup>b</sup>, Placido Neri<sup>b</sup>, Andy Fitch<sup>a</sup>, <sup>a</sup>ESRF, BP 200 - 38043 Grenoble, France, <sup>b</sup>Department of Chemistry, University of Salerno, Italy.

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## Keywords: calixarenes; supramolecular assemblies; synchrotron powder diffraction

At the Dept. of Chemistry of the University of Salerno we prepared and characterized a new crystalline solid based on *p*-Bu'-calix[4]dihydroquinone **1** revealing the simultaneous existence of water channels and very large hydrophobic cavities (988 Å<sup>3</sup>). The compound crystallizes from CHCl<sub>3</sub> and ethylacetate with a cubic structure (a = 36.412(4) Å) containing 48 calixarene molecules and 155 water molecules in the unit cell. The host supramolecular framework is surprisingly robust and that the material behaves as an organic supramolecular zeolite featuring the simultaneous presence of networked