

s7.m25.p1 **Isostructurality in Xanthenol Clathrates.** Ayesha Jacobs¹, Luigi R. Nassimbeni¹ and Benjamin Taljaard².
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Keywords: Clathrates; Isostructurality; Aromatic guests

A series of clathrates comprising the xanthenol host, 9-(4-methoxyphenyl)-9H-xanthen-9-ol, with a variety of aromatic guests displays constant structures in the space group P1.

We have elucidated the structures of the inclusion compounds H·½G, where H is 9-(4-methoxyphenyl)-9H-xanthen-9-ol and G is aniline, benzene, toluene, o-, m- and p-xylene. In all cases the structures crystallise in P1 with a $a \approx 8.373 \text{ \AA}$, $b \approx 9.072 \text{ \AA}$, $c \approx 12.650 \text{ \AA}$, $\alpha \approx 95.470^\circ$, $\beta \approx 96.202^\circ$ and $\gamma \approx 110.315^\circ$. The structures are isostructural with respect to the host and display a consistent (Host) OH...O (Host) hydrogen bonding. The guests lie on a centre of inversion and with the exception of the symmetrical guests, benzene and p-xylene, are disordered. An interesting case arises with m-xylene, which is ordered at low temperature (113 K) with both the host and guest molecules in general positions. At a higher temperature (283 K) the inclusion compound with m-xylene fits the series. We have correlated the structures with the thermal stabilities of the compounds by analysis of their DSC results.

s7.m25.p2 **Structure and Host-Guest Properties of Nanoporous Tetrakisbenzoato diaquacopper(II) Framework Structures with Continuous Channels where Guest Molecules can be Reversibly Incorporated and Released.** Olof Kristiansson, Department of Chemistry, SLU, Box 7015, SE-750 07 Uppsala, Sweden. E-mail: olof.kristiansson@kemi.slu.se

Keywords: Host-guest interactions; Framework structures

$[(p\text{-NO}_2\text{C}_6\text{H}_4\text{COO})_4(\text{H}_2\text{O})_2\text{Cu}_2]$ $((\text{CH}_3)_2\text{CO})$ (**1**) has a Cu-Cu distance is 2.608(1) Å with four p-nitrobenzoate ligands coordinated in a bidentately bridging fashion, with the four bidentately bridging benzoate ligands coordinated in the well-known "paddle-steamer" geometry [1]. It possesses a framework structure with continuous channels parallel to c-axis with an opening size of $\sim 5.6 \times 7.9 \text{ \AA}$, giving a solvent accessible volume of 22 % of the crystal volume. The framework remains intact and crystalline after removal of the included acetone molecule, as determined by X-ray powder diffraction. It is shown, by thermogravimetric measurements, that also benzene and water guest molecules can be reversibly incorporated and released. The framework remains intact and crystalline during these processes. An advantage with the copper(II)benzoate family of compounds is the convenient number of variable parameters to fine-tune the host capabilities. The nature of the aryl ring substituents and axial ligand can be used to optimize the solvent accessible volume, void dimensions or anisotropic properties. Unlike zeolites, these materials not only exhibit hydrophilic properties but also the ability to absorb organic molecules which, together with the possibility of additional substituents on the benzoate molecule to introduce e.g. hydrogen bond capabilities, may enable specific sorptions of a broad range of molecules.

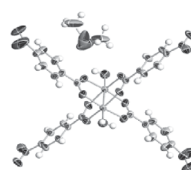


Figure 1. The molecular structure of tetrakis(p-nitrobenzoato) diaquacopper(II) acetone solvate (**1**). Four p-nitrobenzoate groups and two water molecules surround the two Cu^{2+} atoms, giving a square pyramidal coordination. The Cu-Cu distance is 2.608(1) Å.

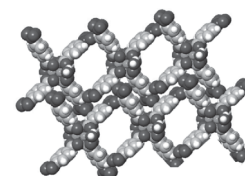


Figure 2. A space filling view of **1** parallel to the c-axis, showing continuous channels with an opening size of $\sim 5.6 \times 7.9 \text{ \AA}$ where acetone, benzene and water guest molecules can be reversibly incorporated and released.

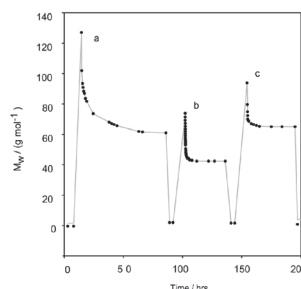


Figure 3. The removal and insertion of guest molecules was examined by heating **1** to 150o to remove the acetone guest molecules, and a subsequent exposure to acetone vapour. This procedure was repeated using benzene and water vapour. The result is shown above, where the molecular weight of the guest molecules is plotted as a function of time. After heating, a minimum weight is obtained corresponding to the empty framework. After exposure to acetone vapour, a weight gain which gradually decreases until a constant weight gain corresponding to 0.98 acetone molecules per formula unit is observed. With benzene and water guest molecules, constant weight was obtained corresponding to 0.79 benzene and 2.27 water molecules. These results conclusively show the reversibility of the guest molecule insertion and removal processes.

[1] O. Kristiansson and L. Tergenius. *J. Chem. Soc. Dalton Trans.* **2001**, 1335.