

alcohol by a coordination polymer involving insertion/de-insertion of the alcohol into a Ag-O(carboxylate) bond will be described.[4] The presentation will further develop the results of recently published work with discussion of ongoing studies of the two systems.

[1] S. J. Delgarno et al., *Chem. Soc. Rev.* 2007, 36, 236.

[2] G. Minguez Espallargas et al., *J. Am. Chem. Soc.* 2006, 128, 9584.

[3] G. Minguez Espallargas et al., *J. Am. Chem. Soc.* 2007, 129, 15606.

[4] S. Libri et al., *Angew Chem. Int. Ed.* 2008, 47, 1693.

Keywords: reactivity of solids, coordination chemistry, hydrogen bonding

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Polymorphism, isostructurality and selectivity in inclusion compounds

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Structures of host compounds with mixed guests are useful in understanding the process of molecular recognition in the solid state. We have elucidated the structures of three polymorphs of the host H1 = 2,2'-bis (hydroxydiphenylmethyl-1,1'-binaphthyl) and a series of its inclusion compounds with pyridine, morpholine and benzene in various proportions. A number of these compounds are isostructural and guests are located at fixed sites in the crystal structures. A second host compound H2 = 9-(2-naphthyl)-9H-xanthen-9-ol was studied in terms of the selectivity towards pairs of guests dioxane/cyclohexanone and dioxane/cyclohexanol. Selectivity profiles are evaluated in terms of the structures of the inclusion compounds with mixed guests. The results were studied by means of triangular diagrams which yielded the stoichiometries of the crystalline inclusion compounds resulting from competition experiments. Structural data is correlated to results of Thermo Gravimetry (TG) and Differential Scanning Calorimetry (DSC) and interpreted via Hirschfeld Surface Fingerprint Plots, lattice energy calculations and host-guest interactions.

Keywords: selectivity, isostructurality, polymorphism

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What are the molecular properties that influence the formation of methanol solvates?

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Despite the considerable scientific interest in solvate crystals, it is generally not possible to predict whether a given molecule will form a solvate when crystallised from a particular solvent. Following a similar account on crystal hydrates [1], the aim of this contribution is the identification of molecular properties that influence the formation of methanol solvates. The Cambridge Structural Database

(November 2007 release, [2]) was searched for molecular organic crystal structures that contain methanol or that are known to be crystallised from methanol. The retrieved structures can be grouped into four main categories: unsolvated crystals, methanol solvates, hydrates and methanol solvate hydrates. Molecular descriptors were calculated for the non-solvent molecules in each group, and statistical methods (t-test, Wilcoxon rank-sum test, Kullback-Liebler divergence) were used to identify the descriptors that best discriminate the four groups. The formation of any solvate was found to depend on the hydrogen bonding functionality of the molecules. Polar surface area and the number of heteroatoms are also useful indicators of solvate formation. The formation of a hydrate from a solution in methanol becomes more likely with increasing molecular polarity (as expressed, e.g., by [nr. of N atoms + nr. of O atoms] / nr. of heavy atoms) and less likely for molecules with a globular shape. The molecules that form mixed solvates are, on average, larger than either methanol solvates or hydrates, they have several hydrogen bonding groups and they are more polar than methanol solvates.

[1] Infantes, L.; Fabian, L. & Motherwell, W. D. S. (2007). *CrystEngComm*, 9, 65-71.

[2] Allen, F. H. (2002). *Acta Cryst.*, B58, 380-388.

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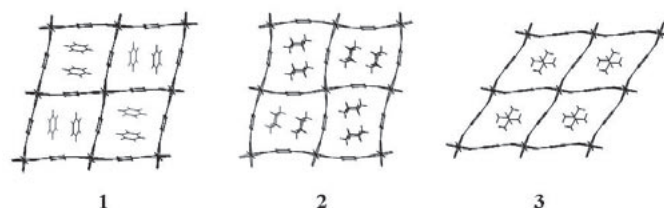
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Framework deformation and guest packing in a microporous vanadium benzenedicarboxylate

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The microporous vanadium benzenedicarboxylate (VOBdc, bdc = 1,4-benzenedicarboxylate) belongs to the third-generation hybrid organic-inorganic materials with flexible or dynamic frameworks that respond to changes in guests and external conditions. The cooperative relations between framework deformations and guest structures in VOBdc loaded with various guest molecules are studied by single crystal X-ray diffraction. The VOBdc framework contains chains of corner-sharing VO₆ octahedra that are cross-linked by bdc ligands. The 1D channels have a diamond shaped section outlined on each side by V-O₂C(C₆H₄)CO₂-V walls. The walls are flat when the channels are empty. Slight bending of the walls toward L shape is observed when the channels are loaded with flat guest molecules such as benzene that are packed in a herring bone pattern, 1. Strong bending of the walls to a C shape is observed when the guest benzene is replaced by bulkier molecules such as cyclohexane, 2, which is in contrast to an S shaped bending of the channel walls when the channels are filled by acetone molecules that are packed in an antiparallel mode, 3.



Keywords: microporous, flexible framework, framework deformation