

interesting characteristics: (a) it has four carboxyl groups that after partial or full deprotonation, can be coordinated to the metal ions in a wide variety of coordination modes leading to high dimensional structures; (b) it can act not only as hydrogen-bond acceptor but also as hydrogen-bond donor, depending upon the number of deprotonated carboxylic groups; (c) its carboxylic groups may not lie in the same plane upon complexation to metal ions owing to geometrical constraints and thus, the ligand may connect metal ions in different directions; (d) finally, its conformation without any phenyl ring gives new possibilities of torsion angles in the structure. All these characteristics make the ligand an excellent candidate to build three-dimensional architectures.

Herein we report the synthesis and X-ray structure of several novel complexes with 1,2,3,4-butanetetracarboxylic acid  $[M_2(\text{but})(\text{H}_2\text{O})_5] \cdot x\text{H}_2\text{O}$  with  $M =$  Transition metals.

**Keywords:** synthesis and characterization of coordination compounds, carboxylic acids, crystal engineering

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#### Supramolecular Isomerism of Three Dimensional 3-connected Coordination Polymers

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Polymorphism and supramolecular isomerism are widely encountered in the crystalline compounds. However, most coordination complexes referred to these concepts contain different guest/solvent molecules. No example has been reported to have supramolecular isomerism in the context of the 3-connected topologies.[1] We have developed a straightforward construction strategy for 3-connected coordination networks.[2] We have also just successfully designed and synthesized four novel supramolecular isomers based on low-dimensional coordination compounds.[3] Here we report three supramolecular isomers based on binary  $\text{Cu}^I$  3,5-dimethyl-1,2,4-triazolate ( $\hat{a}$ ,  $\hat{a}$ ,  $\hat{a}$ ) isolated from different solvothermal conditions. The topologies of  $\hat{a}$ ,  $\hat{a}$ , and  $\hat{a}$  can be rationalized to be  $8^2 10$ - $a$ ,  $4.8.16$ ,  $6.10^2$ , respectively.[2] It should be noted that the 3-connected  $4.8.16$  and  $6.10^2$  nets can also be simplified as 4-connected  $4^2 8^4$  and 6-connected  $\hat{a}$ -Po nets, respectively. The three isomers also display different photoluminescence properties.

[1] Moulton B., Zaworotko M. J., *Chem. Rev.*, 2001, **101**, 1629. [2] Zhang J.-P., Zheng S.-L., Huang X.-C., Chen X.-M., *Angew. Chem. Int. Ed.*, 2004, **43**, 206. [3] Zhang J.-P., Lin Y.-Y., Huang X.-C., Chen X.-M., *Chem. Commun.*, 2005, doi:10.1039/b416095a.

**Keywords:** coordination polymers, supramolecular isomerism, network topology

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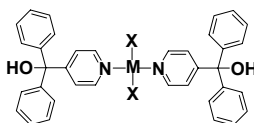
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#### Novel Organometallic Molecular Building Blocks for Crystal Engineering

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Triphenylmethanol (TPM) and its derivatives, for example 4,4'-bis(biphenylhydroxymethyl)biphenyl (DHMB), form chalcate compounds in the solid state [1]. Their crystal structures are usually assembled through host-host  $-\text{OH} \cdots \text{HO}-$  or through host-guest  $-\text{OH} \cdots \text{X}$  interactions[2].

Our current work is addressed to the engineering of crystalline systems combining TPMs interlinked by metal centres structured in porous frameworks, potentially able of hosting small guests. Our approach to the rational design of such architectures is based on the molecular tectonics method, in which the crystal structure is deconvoluted into the contributions of the single inorganic and organic building blocks, which are separately analyzed and optimized. The first step in the modeling of such systems consists in the introduction of a transition



metal as bridge between two aromatic rings. The model ligand studied is  $\alpha$ -(4-pyridyl)benzhydrol (LOH), which combines both the molecular structure of TPMs and the coordinating pyridine functionality. In this work we describe the solid-state organization of  $[\text{M}(\text{LOH})_2\text{X}_2]$  ( $M$ : Pd, Pt, Cu, Zn,  $X =$  halide, acetate) and we correlate the supramolecular arrangement of the organic-inorganic matrix to the stereochemical attitudes of the inorganic component.

[1] Toda F., *Comprehensive supramolecular chemistry*, 6, cap.15. [2] Weber E., Skobridis K., Goldberg I., *Chem. Comm.*, 1989, 1195.

**Keywords:** crystal engineering, coordination compounds, wheel-and-axle

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#### Constitutional Dynamic Self-Amplification in Double-Helix Imine Systems

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Constitutional dynamic chemistry [1,2] expresses adaptative behaviour as its entities are in principle capable of responding to external effectors via reorganization/amplification of their constitution through reversible covalent bonds in order to generate a dynamic functional diversity.

We will present here the ability of a set of imine-metal complexes to undergo such a process in response to the effect of external factors which promote both ligand and imine exchange in order to drive to a constitutional evolution of dynamic mixture toward the selection and amplification of specific components.

From a conceptual point of view these results express a synergistic adaptative strategy for a evolutive generation of crystalline functional devices. Moreover, the self-assembling behaviour of these systems leads to tubular double-helix solid state structures [3]. Different superstructures of this type could be generated by selection and amplification and they will be discussed in detail.

[1] Lehn J.-M., *Proc. Natl. Acad. Sci.*, 2002, **99**, 4763-4768. [2] Barboiu M., Vaughan G., Graff R., Lehn J.-M., *J. Am. Chem. Soc.*, 2003, **125**, 10257-10265. [3] Dumitru F., Legrand Y.-M., Barboiu M., van der Lee A., 2005, *in press*.

**Keywords:** crystal engineering, crystallography, structure

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#### Trisiloxane-Diols and Cyclosiloxanes with Bulky Substituents on the Si Atoms

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A series of siloxane compounds have been synthesized as monomers for the preparation of polymers used as polarisable stationary phases for capillary chromatography [1]. Four trisiloxane-1,5 diols (with different organic substituents on the Si atoms,  $\text{R}_1 = 2$ -methoxybenzene and  $\text{R}_2 = 2,6$ -dimethoxybenzene), have been found to have different configurations of the  $\text{O-Si-O-Si-O-Si-O}$  skeleton. In the crystal structure they are linked to one another by different types of hydrogen bonding. The terminal Si-O distances are significantly longer than the central Si-O distances as reported previously for similar compounds [2].

In a series of cyclosiloxane molecules, containing 3 to 5 SiO units and different organic substituents on the Si atoms ( $\text{Me}$ ,  $\text{Ph}$ ,  $\text{R}_1$ ,  $\text{R}_2$  and  $\text{R}_3 = 2,4,6$ -trimethoxybenzene), it has been shown that the Si-O bond distances and packing of the molecules in the crystal structures are very different, depending on the size of the ring. These features will be discussed in relation to the formation of the polymers.

[1] Monziane M., *PhD thesis*, Université de Neuchâtel, 1995. [2] Graalman O., Klingebiel U., Clegg W. *Chem. Ber.*, 1984, **117**, 2988.

**Keywords:** crystal structure, hydrogen bonding, polymers