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Acta Cryst. (2011) A67, C621**Porous supramolecular compounds based on paddle-wheel shaped copper(II)adenine entities**

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Crystal engineering comprises an understanding of intermolecular interactions that govern crystal packing [1]. Unfortunately, most of the supramolecular networks based on these non-covalent interactions lack the necessary stability required for many potential applications. The ability to create permanent pores in supramolecular solids is considered as one of the biggest challenges in crystal engineering [2]. Usually, formation of a porous solid requires that the network sustaining interactions are of sufficient strength to pay the energetic penalty for existence of the pores themselves.

We report herein the synthesis and crystal structures of two robust isostructural supramolecular porous compounds of Cu(II) and adenine with the formula $[\text{Cu}_2(\text{adenine})_4\text{Cl}_2]\text{Cl}_2 \cdot n\text{CH}_3\text{OH}$ (**1**) and $[\text{Cu}_2(\text{adenine})_4\text{Br}_2]\text{Br}_2 \cdot n\text{CH}_3\text{OH}$ (**2**). They have been obtained using methanol as solvent to assure the direct hydrogen bonding interaction between the adenine ligands, that otherwise would be disrupted by the strong capability of water to mediate such interactions. A handful of covalent 2D and 3D coordination compounds have been reported exploiting the ability of the nucleobases to act as polydentate bridging ligands, as far as we are aware, these compounds represents the first examples of a robust porous 3D architecture based on adenine-containing complexes in which the self-assembling of the structural units is only driven by non-covalent interactions and shows a high thermal stability.

The crystal structure of **1** consists of windmill shaped dimeric complex cations, $[\text{Cu}_2(\mu\text{-adenine})_4\text{Cl}_2]^{2+}$, and chloride counterions. The four bridging adenine molecules are linked to copper(II) ions through its N3 and N9 nitrogen atoms with chlorido ligands in the apical positions providing an elongated square pyramidal coordination environment to the metal centers.

The supramolecular structure involves the direct interaction between the Watson-Crick edges of adjacent adenines to give rise to a 3D overall supramolecular structure containing very large channels with a diameter of ~ 9 Å, that represents 28% of the total volume of the unit cell (Figure 1). The chloride counterions, not being placed inside the channels, contribute to robustness of the crystal structure acting as acceptors from two hydrogen bonds established with the N7 donor positions of two adenine molecules. The crystal structure remains stable up to 200 °C as checked by TG and XRPD measurements.

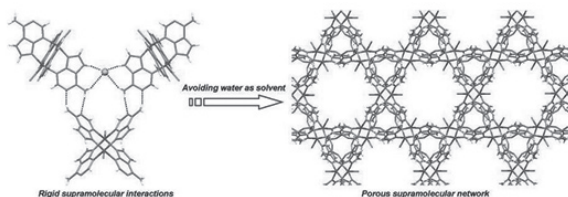


Figure 1. Rigid supramolecular interactions.

[1] B. Moulton, M.J. Zaworotko, *Chem. Rev.* **2001**, *101*, 1629-1658. [2] A.C. Skapski, P. De Meester, *J. Chem. Soc. A* **1971**, *13*, 2167-2169.

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Acta Cryst. (2011) A67, C621**cRy: A Crystallographic Toolbox in R**

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A new library for applications in macromolecular crystallography, called cRy, has been developed in R, the renowned platform for statistical computation. The package allows easy import, manipulation and export of crystallographic data in the most common formats. This is the first software of its kind and is intended to provide a bridge between the large communities of crystallographers and professional statisticians.

Keywords: software, crystallography, statistics

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Acta Cryst. (2011) A67, C621**Linear transformations of variance/covariance matrices**

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We present the application of linear transformations (symmetry operations or changes of the coordinate system) on the variance/covariance matrices of atomic coordinates or of second rank tensors.

Second rank tensors are a very useful concept in crystallography. Probably the most often employed application are the (harmonic) anisotropic displacement parameters in crystal structure refinement. Other important applications are in the description of physical properties, e.g. thermal expansion, strain, etc. Linear transformations on second rank tensors can easily be applied using matrix operations. Many crystallographic programs (PLATON, ORTEP, etc.) have implemented routines to perform this. Less trivial is the application of linear operations to the standard uncertainties. To do this correctly the variance/covariance matrix is necessary. Because most tensors calculations in crystal physics are performed in a Cartesian system, a first step will be a linear transformation from the crystal system to a Cartesian system.

Another related question occurs in the least square refinement of crystal structures: which space group setting is the most suitable? Feast *et al.* [1] argue that a setting with oblique angle increases the correlation between parameters and could give difficulties during the refinement. If the variance/covariance matrix is taken into account for the transformation of the settings, the results of the refinement in the transformed setting can be compared with the transformed results.

[1] G.C. Feast, J. Haestier, L.W. Page, J. Robertson, A.L. Thompson, D.J. Watkin, *Acta Cryst. Section C* **2009**, *65*(12), o635-o638.

Keywords: crystallographic computing, standard uncertainties, linear transformations