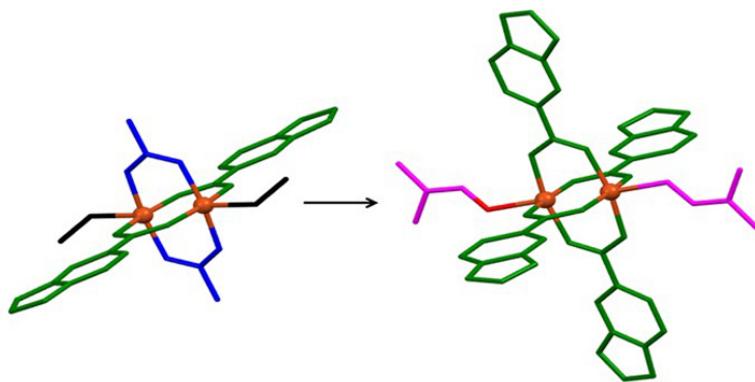


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## Design of new compounds of Cu (II) with carboxylate ligands and pyridines



The synthesis and characterization of different crystalline materials and synthetic biology allow for obtaining porous materials with different metals, such as copper (Cu) or zinc (Zn). Researchers from the UAB have studied the role of carboxylic acids and amines in the structural arrangement in order to design new compounds of Cu (II) with carboxylate and pyridine ligands. This has allowed them to know both the molecular structure and the supramolecular structure and, therefore, to increase the knowledge about the state of the art.

Supramolecular chemistry is an emergent research area that provides new complexes. These systems are composed of two or more assembled molecular units, which are connected by covalent bonds or weak intermolecular forces (hydrogen bond, van der Waals forces, and electrostatic effects, among others).

The synthesis and characterization of crystalline materials build up covalent bonds has gained interest in recent years, in particular the assembly of metal-carboxylates. These kind of compounds play an important role in synthetic chemistry for the design of porous materials with different metals as Cu(II) and Zn(II).

Recently, our research team has been studying the role of carboxylic acids and different amines

in the structural arrangement.

In this work, we aimed to design new compounds of Cu(II) with carboxylate ligands (XCCO-) and pyridine/pyrazole ligands. The result obtained indicated the importance of the initial compound in the nuclearity of final compound (mononuclear, binuclear). We have synthesized and characterized six compounds; four are monomers and two dimers. All compounds were obtained from same initial compound. These six compounds were characterized by analytical, spectroscopic and single crystal X-ray diffraction.

This study allows to know the molecular and extended structures, obtaining 1D and 2D supramolecular networks. One of the monomers obtained shows in their structure three methanol and one occluded water molecules. The solvent accessible volume of the channels is a 6.2% of the cell volume. Under air exposure, the guest solvent is lost. Unfortunately, these changes seem to provoke the collapse of the pores, and the material does not absorb any significant amount of nitrogen.

Finally, for all these compounds, the UV-Vis spectra has been recorded, analyzed and compared with the spectra of other compounds described in the literature.

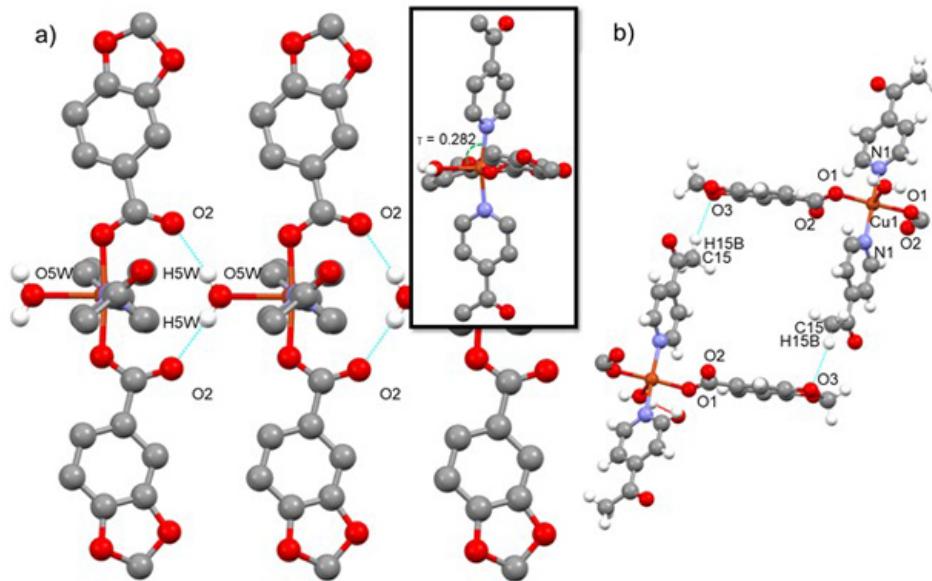


Figure 1. a) View of the one-dimensional ordering of one compound. b) Molecular structures of two compounds.

**Josefina Pons Picart**

Inorganic Chemistry area

Department of Chemistry

Universitat Autònoma de Barcelona

[Josefina.Pons@uab.cat](mailto:Josefina.Pons@uab.cat)

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