

**Figure 1.** The ambient pressure structure of CuPyr-I viewed perpendicular to the *a*, *b* face. This is a one-dimensional porous material with large channels 9 Å in diameter at their widest point, shown in the figure by the orange spheres.

**Keywords:** MOF, High Pressure, Phase Transition

## MS37-P10 Crystal structures of novel polydentate N,O-ligands

Stanislava Todorova<sup>1</sup>, Vanya Kurteva<sup>1</sup>, Boris Shivachev<sup>2</sup>, Rositsa P. Nikolova<sup>2</sup>

1. Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 9, 1113 Sofia, Bulgaria

2. Institute of Mineralogy and Crystallography "Acad. Ivan Kostov", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 107, 1113 Sofia, Bulgaria

email: stodorova@orgchm.bas.bg

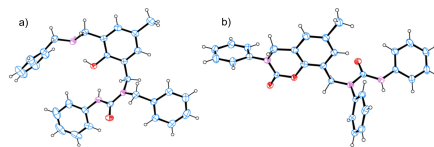
Polydentate molecules are of growing interest as they are widely applied as scaffolds in the combinatorial synthesis of artificial receptors for ions with medical and environmental potential. Among the broad variety of synthetic molecules, polyazaoxa ligands have received special attention due to their outstanding coordination abilities. A particular goal involves the construction of ligands with an appropriate order and predictable arrangement of two or more molecular components with possibility to form hydrogen bonds, which play the pivotal role in molecular recognition by synthetic receptors.

Herein, we present a study on the crystal structures of a series of novel polydentate N,O-ligands possessing unsymmetrical urea fragments attached to a *p*-cresol scaffold. The compounds are obtained by a fast and simple protocol from *p*-cresol-based symmetrical bis-amine, phosgene, and primary amine. Their structures are assigned by 1D and 2D NMR spectra in solution and by single crystal XRD in solid phase. Ortep drawings of selected crystal phases are presented on Figure 1.

The ligands can be generally divided in two groups: open-chain substituted aromatics with at least one unsymmetrical urea unit (a) and fused aryloxazinones with unsymmetrical urea fragment (b). The concept is to design polydentate ligands with variable coordination abilities controlled by the difference in the molecule geometry.

The single crystal XRD analysis showed that the open-chain substituted molecules are oriented towards optimal intramolecular H-bonding of the ureas' heteroatoms, while the preferred geometry of oxazinones is driven by intermolecular bonding.

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**Figure 1.** ORTEP drawings of selected samples

**Keywords:** polydentate N,O-ligands , singal crystal XRD