

## MS36-P11

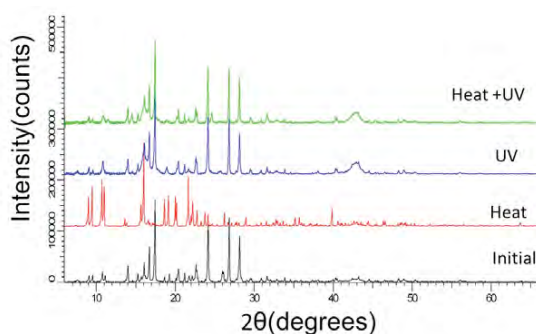
## Effect of dehydration on zinc malonate complexes with 1,2-bis(pyridin-4-yl)ethylene

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Recently we carried out a series of photoinitiated reactions in zinc malonates with bis(pyrid-4-yl)ethylene [1]. The transformation of  $\{[\text{Zn}(\text{bpe})(\text{Me}_2\text{mal})]\cdot\text{H}_2\text{O}\}_n$  to  $\{[\text{Zn}(\text{bpe})(\text{Me}_2\text{mal})]_2[\text{Zn}_2(\text{tpcb})(\text{Me}_2\text{mal})_2]\cdot\text{H}_2\text{O}\}_n$  ( $\text{Me}_2\text{mal}$  = dimethylmalonate,  $\text{tpcb}$  = 1,1,2,2-tetrakis(pyridine-4-yl)cyclobutane) was proposed to be affected by dehydration reaction. Thus, we studied the effect of dehydration on above  $\{[\text{Zn}(\text{bpe})(\text{Me}_2\text{mal})]\cdot\text{H}_2\text{O}\}_n$  and its isostructural analog  $\{[\text{Zn}(\text{bpe})(\text{cbdc})]\cdot\text{H}_2\text{O}\}_n$  ( $\text{cbdc}$  = cyclobutane-1,1-dicarboxylate). Both compounds were heated for 2 hours at 120°C until constant weight and then irradiated with UV for 8 hours. Transformations of crystalline compounds were controlled by means of powder X-ray diffraction (Figure) and <sup>1</sup>H NMR. As it follows from Figure, similarly with  $\{[\text{Zn}(\text{bpe})(\text{Me}_2\text{mal})]\cdot\text{H}_2\text{O}\}_n$  dehydration of  $\{[\text{Zn}(\text{bpe})(\text{cbdc})]\cdot\text{H}_2\text{O}\}_n$  to  $\{[\text{Zn}(\text{bpe})(\text{cbdc})]\}_n$  and irradiation of the latter compound can be described as a two-stage solid-state process. Based on our data, irradiation of  $\{[\text{Zn}(\text{bpe})(\text{cbdc})]\cdot\text{H}_2\text{O}\}_n$  at room temperature seem to be accompanied by dehydration. Analysis of the reaction products is underway now.



## References:

- [1] Ekaterina N. Zorina-Tikhonova et al., (2018) IUCrJ, 5 2052-2525.

Keywords: photoinitiation, complex compounds, X-ray diffraction

## MS36-P12

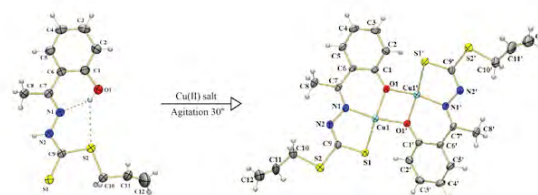
## Structural analysis and antimicrobial activity of a new dithiocarbazate and its Copper(II) complex

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Dithiocarbazates and their metal complexes have been the subject of many studies because they have a wide range of pharmaceutical applications and also because of their chemical and structural versatility.<sup>[1,2]</sup> These Schiff bases present themselves in their varied structures coordination sites and allow the formation of complexes with several transition metals. Based on our interest in this class of compounds, the present study describe the synthesis and crystallography evaluation of the new ligand 2-hydroxyacetophenone-S-dithiocarbazate (**H<sub>2</sub>L<sup>1</sup>**) and its copper(II) complex, **[(CuL<sup>1</sup>)<sub>2</sub>]**. The compounds were characterized by elemental analysis and spectral measurements (IR, UV-Vis, <sup>1</sup>H NMR and <sup>13</sup>C NMR). The packing architectures revealed by single crystal X-ray diffraction analysis showed bifurcated intramolecular hydrogen bonds which are responsible for the formation of a dimer-like structure. The ligand adopts an *E* configuration and tautomeric and thione form. The copper(II) complex is a dimeric structure with a distorted square planar coordination geometry around each copper atom. The metal centers are connected by  $\mu_2$ -oxo bridges with *ONS*-donor ligands. The distance between the metal atoms of is 2.926(6) Å, long enough to have any metal-metal interaction. In addition, the biological properties of the compounds were evaluated against a variety of bacteria and fungi. In all experiments, due the structure and properties of the copper(II) complex was a greater antimicrobial activity observed compared to the free dithiocarbazate.



## References:

- [1] Zangrando, E. et al. (2015). Inorg. Chim. Acta. 427, 278-284.  
[2] Mirza, A. H. et al. (2014). Polyhedron. 81, 723-727.

Keywords: Crystallography, Dithiocarbazates, Biological Analysis