

MS43-P7 **Synthesis, Crystal Structure and Thermal Behavior of Coordination Polymers Based on Zinc(II).** Eva Fernández-Zapico,^a Jose Montejo-Bernardo,^a José R. García,^a Santiago García-Granda,^a *Departments of Physical and Analytical Chemistry and Organic and Inorganic Chemistry, University of Oviedo - CINN, Spain*
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Three non-isostructural zinc(II) coordination polymers were synthesized (varying the time of reaction or the molar ratio of reagents) under mild hydrothermal conditions ($T = 140^\circ\text{C}$) by mixture of zinc(II) acetate with 2-carboxyethylphosphonic acid and 1,10'-phenanthroline. All products were obtained as colorless single-crystals, but with different morphology. Their structures were determined by single-crystal X-ray diffraction, and the corresponding thermal stability is studied. Compound $[\text{Zn}_2(\text{HO}_3\text{PCH}_2\text{CH}_2\text{COO})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]$ (**ZnPF1**) is monoclinic (space group $P2_1/c$) and crystallizes as discrete dimeric molecules, with one water molecule coordinated to each Zn atom, similarly to a previous reported structure [1]. Compound $[\text{Zn}_5(\text{HO}_3\text{PCH}_2\text{CH}_2\text{COO})_4(\text{C}_{12}\text{H}_8\text{N}_2)_4(\text{H}_2\text{O})_{0.32}]$ (**ZnPF2**) is also monoclinic (space group $C2/c$) and crystallizes as a tridimensional network, presenting channels in which water molecules are placed. One peculiarity of this compound is the presence of three different Zn atoms (four-five-six coordinated) in their structure. Although there are some examples in the literature which shows this feature [2-6], all of these consist in discrete molecules. Here we present the first tridimensional coordination polymer (MOF) with three Zn atoms having different coordination number. Compound $[\text{Zn}_6(\text{HO}_3\text{PCH}_2\text{CH}_2\text{COO})_2(\text{C}_{12}\text{H}_8\text{N}_2)_1(\text{H}_2\text{O})_2]$ (**ZnPF3**) is triclinic (space group $P-1$) and crystallizes forming 2D layered packing, with water molecules located in channels along a -axis. This compound also presents three different Zn atom in the structure (four-four-six coordinated). For these three compounds, structural features, including H-bond network and the π - π stacking interactions were reported and discussed here.

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MS43-P8 **Understanding hybrid polymeric materials with *N*-salicylidene aniline derivatives: a structural approach.** Pierre-Loïc Jacquemin,^a Koen Robeyns,^a Jacqueline Marchand-Brynaert,^a Michel Devillers,^a Yann Garcia,^a *Institute of Condensed Matter and Nanotechnology, Université catholique de Louvain, Belgium,*
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N-salicylidene aniline (SA) derivatives belong to one of the rare families of molecules that present photochromism and thermochromism in the solid state [1]. Thermochromism is due to a tautomeric equilibrium between the white enol form and the yellow *cis*-keto form. The photo-isomerisation that occurs between the yellow *cis*-keto and the red *trans*-keto form is responsible of photochromism. Our project concerns the study of hybrid materials prepared by the insertion of anionic SA [2] into a polymeric matrix, synthesized by radical polymerization between substituted diallylamine and maleic acid, that presents an interesting lamellar structure [3]. Those hybrid materials represent remarkable systems for the study of host-guest interactions.

A novel structural approach was recently designed for the study of these systems. More than six salts of substituted diallylamine with *N*-salicylidene aniline sulfonate, which display interesting thermo- and photochromic properties, were crystallized. As an example, diallylhexylammonium-*N*-salicylidene 4-aniline sulfonate crystallizes in a monoclinic space group ($P2_1$). One intra-molecular H-bond is observed between the imine and the enol functions. Other H-bonds, in addition to an ionic interaction, connect the anion to the neighboring diallylhexylammonium that maintain the crystal packing organization. This anion presents a very high stability for the photo-induced *trans*-keto form which is formed in crystal cavities.

This large library of crystal structures helped us to propose a realistic insertion model in hybrid matrices based on the complete description of structural properties. This new structural approach is helpful for the understanding of hybrid polymeric materials with long lateral alkyl chains.

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