MS30-P10 New copper(II) halogenobenzoate complexes with nicotinamide: isomerism and supramolecular structure

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Nicotinamide (nia) has been employed as a supramolecular reagent [1,2]. Some copper(II) carboxylate complexes have shown that the intermolecular H-bonds can alter their magnetic properties. We have recently published mononuclear molecular complex [3] and binuclear molecular complex [4]. which exhibit similar magnetic properties. These very similar magnetic properties of mononuclear as well as binuclear complexes could be explained by the presence of very similar H-bond systems, supramolecular synthons, that are pathway for antiferromagnetic interactions. In this report we present various crystal structures of new copper(II) halogenobenzoate complexes with nicotinamide of formulas $[Cu(X\text{-}bz)_2(nia)_2]$ and $[Cu(X\text{-}bz)_2(nia)_2(H_2O)_2]$. The two polymorphs of $[Cu(2,6\text{-}Cl_2bz)_2(nia)_2]$ are examples of coordination compounds, which are conformation and supramolecular isomers. Additionally, the $[Cu(X\text{-}bz)_2(nia)_2(H_2O)_2]$ and $[Cu(X\text{-}bz)_2(nia)_2]\bullet 2H_2O$ present examples of coordination isomerism. The molecules of all compounds are connected by N—H•••O and/or O—H•••O hydrogen bonds from NH_2 groups of nicotinamide and water molecules, which create supramolecular hydrogen-bonding-coordination chains and networks.

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Keywords: nicotinamide, isomerism, hydrogen bonds, copper(II) benzoate

MS30-P11 Tailoring supramolecular assemblies of β-diketonato Co(II) and Ni(II) complexes

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In order not to rely on serendipity when targeting a desired physical property, we need an improved understanding of how metal-complexes can be organized and assembled into 3D solids using relatively weak and reversible interactions. Certain supramolecular synthons have already proved to be promising and reliable tools in engineering of crystalline organic substances. To examine the robustness and reliability of those synthons in metal-organic systems we have opted for β-diketonato complexes. β-Diketonates are a promising class of chelating ligands that eliminate the need for involvement of additional anions into the building of supramolecular assemblies. In this way, the functionalities are not exposed to the (usually) disruptive nature of counter ions commonly encountered in metal-organic systems, and are expected to communicate and interact with each other in the same manner as they do in purely organic systems. Nevertheless, the outcomes of our best theoretical and experimental efforts are often surprising.

Here, we report on a series of β-diketonato complexes of Co(II) and Ni(II) with selected structure directing N-heterocyclic ligands with the intention of giving an insight into the requirements that have to be met by the ligand itself, as well as by the complex as a whole, for the expected supramolecular behaviour to be achieved. The data are complemented by CSD data mining and extensive computational methods are used to facilitate the interpretation of the experimental efforts.

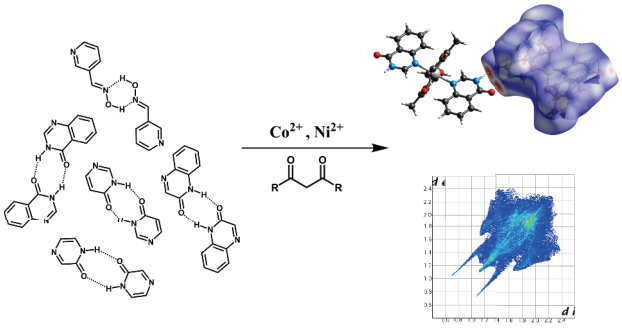

Figure 1. From selected ligands to final products and results.

Keywords: Metal Complexes, Crystal Engineering