Oral presentation

Isostructurality, supramolecular isomerism, and single-crystal-to-single-crystal transformations in a family of metal complexes with a new bipodal ligand

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Research on metal complexes has enjoyed unflagging interest for decades due to their high structural diversity and broad applications. The exploration of this group of compounds intensified even more when the possibility of obtaining materials of predefined structure and particular properties was revealed for a subgroup of very diverse coordination polymers, with applications (among others) in gas storage, catalysis or ion exchange [1]. However, isoreticular syntheses are rather rare and don't always lead to homogeneous products. External factors like temperature, solvent, pH, or concentration can affect the formation of the final products [2-3]. Moreover, supramolecular isomerism [4], driven by the interplay of intermolecular interactions, can also have a final surprise in store. This could be easily overlooked without further SC/PXRD structural studies [5]. The former method is very useful, not only to uncover the structures of products, but also in selected cases to follow externally triggered transformations taking place in the crystal unity [6-7].

In continuation of our ongoing studies on the influence of external factors on the formation of particular coordination architectures and dynamics taking place in the crystal unity, we would like to present a series of five novel transition metal complexes with the ligand 2,6-bis((2-methylimidazol-1-yl)methyl)naphthalene. We isolated two isostructural Cd(II) and Cu(II) coordination polymers, as well as two Co(II) supramolecular isomers, showing polymeric (1D) or discrete (0D) structures, respectively. Furthermore, we were able to follow changes at the molecular and supramolecular level, caused by solvent removal from the latter system, 'in situ' as the transformation took place in a single-crystal-to-single-crystal fashion. The details of these findings will be presented.

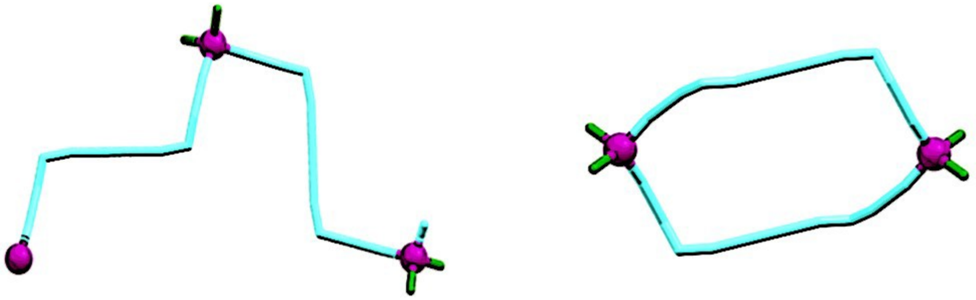

Figure 1. Simplified representation of isolated supramolecular isomers: a fragment of a polymeric 1D chain (on the left) and a discrete 0D Co(II) metal complex (on the right).

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