Poster Presentation

MS035.P16

Influence of synthetic conditions on the structures of cadmium complexes

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In the crystal engineering, the design of self-assembled coordination networks is affected by control of the directional and non-directional noncovalent interactions such as hydrogen bonding, halogen bonding and π-based interaction. It is well known that selection of ligand and metal type as building blocks in the coordination compounds have an important role in the construction of final crystal architecture. Moreover, the reaction conditions such as temperature, reaction time, reagent ratio, pH, counter ion and solvent are major factors for determination of products. In this regard, applying the various synthetic methods can be driving force to prepare different product using same starting reagents. In this study, the effect of different synthetic routes based on the solution and solid state conditions on the final products were investigated. Consequently, the colorless block crystals were obtained by the double-layered diffusion method (complex 1), while the solvent-free conditions resulted in the yellow powder sample (complex 2). In presence of N-(thiazol-2-yl) pyrazine-2-carboxamide ligand and cadmium (II) iodide reagents in a 1:1 ratio, titled complexes were synthesized and structurally characterized by IR spectroscopy, CHNS elemental analyses, powder and single crystal X-ray diffraction analysis. The coordination environment of cadmium ion in solution-based compound (1) consists of two iodine ions and two different carboxamide ligands which has the distorted square pyramidal geometry with a trigonality index, τ5 of 0.04. The structural investigation of (1) clearly illustrates the amide hydrogen atom transfer to the nitrogen atom of thiazole ring which occurs only for one of coordinated ligands. The structure determination of solid-state based compound (2) from powder diffraction data emphasizes to the different structural motif of cadmium complex in the crystal packing.

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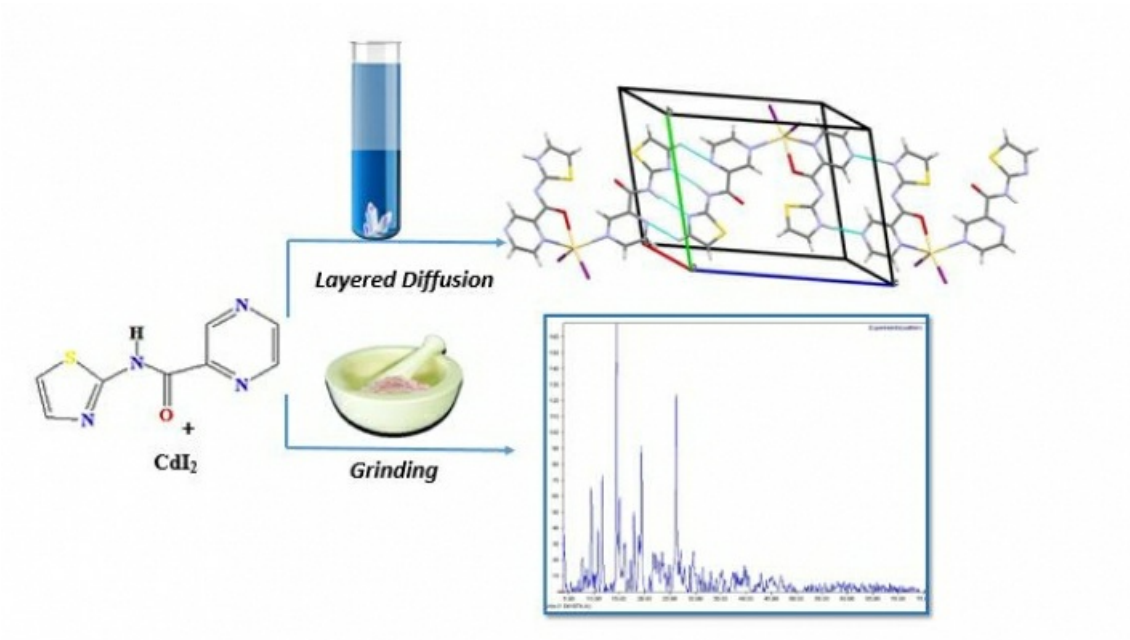

Keywords: solvent-free reactions, proton transfer, noncovalent interaction