

**MS13-2-15 The synthesis and crystal structure of novel coordination polymers of cadmium(II) with hexamethylenetetramine ligand**  
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**Abstract**

Supramolecular chemistry is of great interest not only because of the rich architectural variety of compounds but also their unusual properties. Crystalline coordination polymers could have the potential application as molecular absorbents [1], heterogeneous catalysts [2], optical materials [3], gas storage substrates [4] and many more.

The most important element in the design of metal-organic crystalline phases is the choice of appropriate building blocks which symmetry and the ability to create specific interactions have a significant impact on the final product.

High symmetry ligands such as hexamethylenetetramine (hmt, urotropine) are of great significance to the design of novel metal – organic compounds. Urotropine has a considerable potential for application as a building block because of the four nitrogen atoms which are the metal ions coordination points and give the ability to create different coordination modes spanning from terminal monodentate to bridging bi-, tri-, and tetradentate. The topological features of urotropine and possibility of creating numerous intermolecular interactions increase the probability of obtaining coordination polymers with one-, two-, and three-dimensional networks [5,6]. Divalent cadmium ions are one of the most commonly used metal ions in the design of coordination polymers due to their stable  $d^{10}$  closed-shell electron configuration. The associated absence of ligand field stabilization energy creates a specific coordination environment, ideal for the steric requirements imposed by a particular organic ligand. The lack of allowed d-d transitions facilitates optical properties such as luminescence [6,7] or, in the case of non-centrosymmetric compounds, provides a wide window for second harmonic generation experiments [8].

The result of this research are three novel multicomponent chemical compounds:  $[\text{Cd}(\text{hmt})_2(\text{H}_2\text{O})_2\text{Br}_2]$  (**1**),  $\{\text{Cd}_2(\text{hmt})(\text{H}_2\text{O})_2\text{Br}_4\}_n$  (**2**),  $\{\text{Cd}_2(\text{hmt})(\text{DMF})\text{Br}_4\}_n \cdot 2n(\text{DMF})$  (**3**). Two of them are coordination polymers with two- (**2**) and three-dimensional network (**3**). These products were obtained by the reaction of urotropine with cadmium bromide in the presence of three different solvents: isopropanol (**1**), ethanol (**2**) and N, N - dimethylformamide (DMF) (**3**). The interesting structural motifs stabilized by numerous hydrogen bonds are observed in the obtained coordination polymers. Hirshfeld surface analysis was applied to analyze the differences between the intermolecular interactions in obtained compounds.

**References**

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Crystal structure of obtained compounds:1, 2, 3.

