

acid affects its coordination ability and in compound **2** the ligand only connects to the metal by the carboxylate group. In the structure it is observed a dimetallic subunit where the Zn atoms are bonded by three ligands. These units are linked by another ligand through its carboxylate fragment, rendering a disposition where the metals are bonded to four oxygen atoms in a tetrahedral geometry.

[1] I.R. Amiraslanov, G.N. Nadzhafov, B.T. Usuballiev, A.A. Musaev, E.M. Movsumov, Kh.S. Mamedov. *Zh. Strukt. Khim*, **1980** 21(3), 140. [2] A. Millward, O.M. Yaghi, *J. Am. Chem. Soc.*, **2005**, 127, 17999. [3] Jesse L.C. Rowsell, O. M. Yaghi, *Microporous and Mesoporous Materials*, **2004**, 73, 3–14.

Keywords: carboxylate, coordination, zinc

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Design and crystal structures of novel lamotrigine cocrystals

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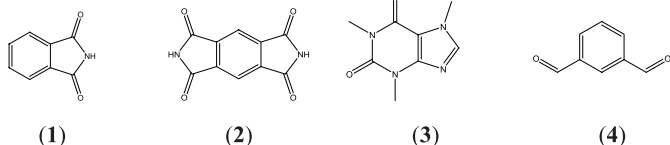
Design of cocrystals is conducted with detailed examination of selected API (Active Pharmaceutical Ingredient) molecular fragments that can be involved in supramolecular assemblies as well as with analysing similar structures available in crystallographic data bases. Exploring the potential of cocrystal formation contributes for better understanding the basic principles of supramolecular chemistry.

In this work, lamotrigine, an antiepileptic drug was chosen as a model drug to design and prepare cocrystals on the basis of the synthon types and interactions found in its crystalline structures of salts and solvates. Due to its basicity, nitrogen N2 atom of triazine ring is always protonated in lamotrigine salts.

It is well known that the N-H...N hydrogen bonds between amino groups and the N2 triazine nitrogen atom form an $R_2^2(8)$ dimer in lamotrigine structure itself [1]. These dimers are usually further connected via N-H...O hydrogen bonds between another N-H amino group and oxygen atoms of oxygen containing solvate molecules into more complex hydrogen-bonded rings.

These synthons along with the presence of chlorine atoms in lamotrigine molecule are considered as models in design of targeted lamotrigine cocrystals.

In that context, four cocrystal former molecules are chosen for lamotrigine cocrystal preparation: phthalimide (**1**) and analogous pyromellitic diimide (**2**), caffeine (**3**) and isophthalaldehyde (**4**) on the basis of their stereochemically disposable proton donors (N-H) and proton acceptors (keto groups). In cocrystal structures with (**1**), (**2**) and (**3**) molecules, the lamotrigine N-H groups and the triazine N2 atom participate into hydrogen bond formation mutually via N-H...N hydrogen bonds and with cocrystal molecule via N-H...O=C bonds. The presence of the Cl...O short contacts in (**2**), (**3**) and (**4**) structures has been confirmed.



[1] B. Sridhar and K. Ravikumar, *Acta Cryst.* **2009**, C65, o460-o464.

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Synthesis and structural analysis of cadmium dipicolinate coordination polymers and tetramers

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Metal coordination polymers constructed with multi-carboxylate ligands have been extensively studied in supramolecular chemistry and materials chemistry due to their structural diversity and application in catalysis, ion exchange, adsorption, nonlinear optics, luminescence and magnetism. [1] Dipicolinic acid, dipicH_2 , is a versatile chelating ligand which can interact with metal ions both in anionic and protonated form. It is widely used for the preparation of the various metal complexes. It displays a large number of coordination modes due to the position of its carboxylate groups and its nitrogen atom, with the potential to act as a bidentate, tridentate and/or bridging ligand [2].

Here we report the hydrothermal preparation of two cadmium dipicolinate polymers and four tetramers. The two polymers have the formula $[\text{Cd}_2(\text{H}_2\text{O})_3(\text{dipic})_2]_n$ and are polymorphs of each other. The four tetramers can be classed into two groups of general formula $[\text{Cd}_2\text{X}(\text{H}_2\text{O})_4(\text{dipic})(\text{dipicH})]_2 \cdot 2\text{H}_2\text{O}$ and $[\text{Cd}_2\text{X}_2(\text{H}_2\text{O})_3(\text{dipicH})_2]_2 \cdot 2\text{H}_2\text{O}$, where X = Cl or Br. The structures of the compounds have been elucidated by single X-ray diffraction and their thermal behaviour characterized by thermal gravimetry and differential scanning calorimetry.

Using either the cadmium bromide or chloride salt in a 1:1 ratio with dipicolinic acid can lead to any of the above type of structures, indicating the importance of subtle differences in preparation conditions, e.g. concentration of reactants and duration of heating.

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Structural analysis of hexa-imidazole cobalt (II) 2-bromide tetrahydrate

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Hexa-imidazole cobalt (II) 2-bromide tetrahydrate, formulated as $\text{C}_{18}\text{H}_{32}\text{Br}_2\text{CoN}_{12}\text{O}_4$ (I), was synthesized. The crystal and molecular structure of (I) have been determined by X-ray single crystal diffraction. The compound (I) crystallizes in the triclinic, space group P-1 with unit cell parameters $a=8.8660(8)\text{Å}$, $b=9.2117(9)\text{Å}$, $c=10.7641(10)\text{Å}$, $\alpha=76.356(8)^\circ$, $\beta=83.275(8)^\circ$, $\gamma=61.527(7)^\circ$, $R_1=0.431$, and $wR_2=0.0993$.

The title compound is composed of $[\text{Ni}(\text{imidazole})]^{2+}$ complex cations, Br atoms and water molecules. The cobalt atom is located at special positions. The Co atom has octahedral coordination geometry defined by imidazole rings coordinated through N atoms.

The crystal packing is achieved by strong and moderate hydrogen bonds which play an important role in the formation of the 3D network.