

# SUPRAMOLECULAR SODIUM CAVITANDS BASED ON COMPLEXES OF COBALT (II) AND NICKEL (II) WITH 2-(PHOSPHONOMETHYL)AMINOSUCCINIC ACID

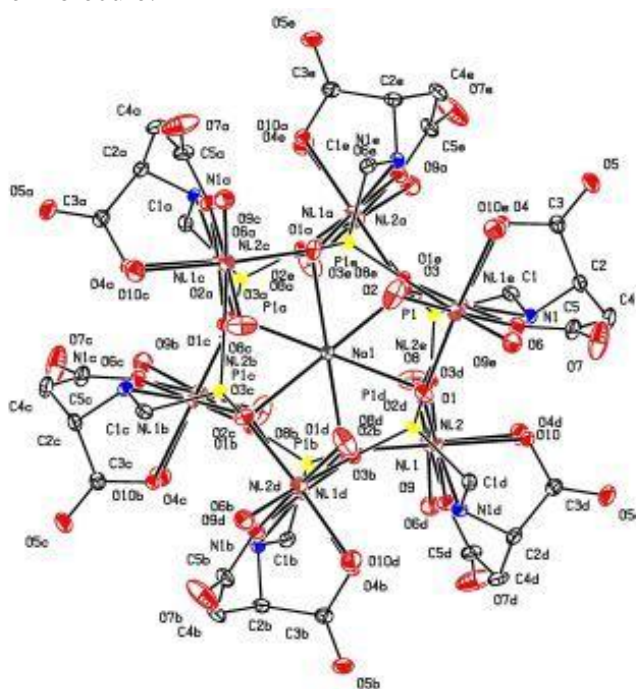
*Anatoliy I. Gerasimchuk, Ganna V. Shovkova, Andriy O. Gudima, Olena K. Trunova*  
[gerasimc@bigmir.net](mailto:gerasimc@bigmir.net) - V.I. Vernadskii Institute of General and Inorganic Chemistry of the Ukrainian National Academy of Sciences, Ukraine, 03680 Kyiv 142, Akademika Palladina Ave. 32/34

One of the most important challenge of supramolecular chemistry is preparation and study of new polymeric network coordination compounds, where metal cations inter-connected by organic bridging ligands. Recent decades display growing interest to the complexes based on mixed carboxylate-phosphonate ligands, due to their potential use in catalysis, photochemistry, ion exchange, intercalation chemistry, etc.

Two novel isostructural metal complexes with 2-(phosphonomethyl)aminosuccinic acid,  $\text{H}_2\text{O}_3\text{PCH}_2\text{NCH}(\text{CO}_2\text{H})\text{CH}_2\text{CO}_2\text{H}$  ( $\text{H}_4\text{PMAS}$ ) namely  $\text{NaM}_{12}(\text{PMAS})_6(\text{OH})(\text{H}_2\text{O})_{17}$  (where  $\text{M}=\text{Co}(\text{II})$  (**1**) or  $\text{Ni}(\text{II})$  (**2**)), have been synthesized. from aqueous solutions upon slow evaporation.

Complexes **1** and **2** crystallize in the rhombohedral crystal system (space group  $R\bar{3}$ ) with 1/6 of the molecule in the independent unit with cell parameters for **1**:  $a = 13.4686(2) \text{ \AA}$ ,  $\alpha = 104.1860(10)^\circ$ ; for **2**:  $a = 13.3789(2) \text{ \AA}$ ,  $\alpha = 103.81^\circ$ . Crystal structure of investigated compounds shows complicated 3D network of hydrogen bonds.

The molecular structure of isomorphous 12-nuclear compounds contains 24-membered macrocycle creating tunnel type cavity comprising the octahedrally coordinated sodium atom, which occupies a special position on the three-fold axis and is inversion centre of the molecule.



Atom Na(1) forms a distorted octahedral environment. All Na-O distances are the similar for the complexes **1** and **2** and of 2.428 (3) Å and 2.433 (2) Å respectively.

The geometry of the void is calculated as a cylinder with generatrix, which contains Na(1) atom and coincides with 3-fold axis. The cavities have a cylindrical shapes with diameters of 6.208 Å and 6.136 Å for compounds **1** and **2** respectively. The heights of the cylinders are of 7.705 Å and 7.589 Å values for **1** and **2** ; the cavity's volumes are 233.1 and 224.3 Å<sup>3</sup> for the complexes **1** and **2**.

These results open a perspectives for use of 3d-metal complexes with 2-(phosphonomethyl)aminosuccinic acid and its analogs as effective alkali metal cavitands, gas absorbents, magnetic materials, new sorbents and other applications.