Synthesis, Characterization, and Crystal Structure of A Novel 2D Metal Diphosphonate: Cu$_3$[C$_6$H$_{20}$N$_2$O$_{14}$P$_4$].2H$_2$O

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Metal diphosphonates are attractive for the diversity structures range [1] from zero-dimensional cages, one-dimensional chains, two dimensional layers to three-dimensional frameworks and potential applications as catalysts, molecular sieves, non-linear optical materials and magnetic materials [2].

As part of our current studies [3] Hydrothermal reaction of N-methyl-iminobis(methylene phosphonic acid), CH$_3$N(CH$_2$PO$_3$H$_2$)$_2$, (H$_4$L) with copper(II) acetate lead to a new layered Cu(II) amino diphosphonate, namely, Cu$_3$(HL)$_2$ (1). The X-ray crystallographic determination reveals copper ions in two different coordination environments. The Cu1 atom has a distorted square pyramidal geometry, whereas the Cu2 atom has a distorted elongated tetragonal octahedral geometry. The HL trianion acts as a pentadentate ligand with deprotonated nitrogen atom and two oxygen atoms of each phosphonate group binding to metal ion. Hydrogen bonds between lattice water molecules in interlayer spaces and the non-coordinated phosphonate oxygen atoms as well as aqua ligands lead to a three-dimensional supramolecular network structure.

A mixture of H$_4$L (0.52 mmol, 0.104 g), Cu(OAc)$_2$.H$_2$O (0.52 mmol, 0.114 g) in deionized water (5.0 mL), adjusted to pH = 5 was sealed in a 20 mL teflonlined stainless steel autoclave, and then heated at 140 °C for 5 d. After the mixture was slowly cooled to room temperature, blue crystals were filtered off, washed with distilled water, and dried at room temperature (yield: ca. 43 % based on Cu). The structure of this complex were characterized from their elemental analysis, IR, and TGA and X-ray crystallography.

REFERENCES