

SYNTHESIS, STRUCTURAL CHARACTERIZATION AND TOPOLOGICAL ANALYSIS OF A TWO DIMENSIONAL COBALT(II) COORDINATION POLYMER WITH 5-(DIHYDROXYPHOSPHORYL)NICOTINIC ACID

Magdalena Wilk¹, Jan Janczak² and Veneta Videnova-Adrabinska¹

¹*Department of Chemistry, Wrocław University of Technology,
27 Wybrzeże Wyspiańskiego St., 50-370 Wrocław, Poland*

²*Institute of Low Temperature and Structure Research, Polish Academy of Sciences,
2 Okólna St., 50-422 Wrocław, Poland
e-mail: magdalena.wilk@pwr.wroc.pl*

A novel cobalt(II) coordination polymer has been synthesized and structurally characterized by a single-crystal X-ray diffraction method. $[\text{Co}_2(\text{L})(\text{H}_2\text{L})(\text{H}_2\text{O})_3]_{2n}$, where H_3L is 5-(dihydroxyphosphoryl)nicotinic acid, crystallizes in the triclinic crystal system with a space group $P\bar{1}$. The unit cell parameters are: $a = 5.112(1) \text{ \AA}$, $b = 13.620(2) \text{ \AA}$, $c = 14.589(3) \text{ \AA}$, $\alpha = 62.82(2)^\circ$, $\beta = 84.24(1)^\circ$, $\gamma = 84.99(1)^\circ$, $V = 898.1(3) \text{ \AA}^3$ and $Z = 2$. The asymmetric unit consists of two independent Co(II) ions, one monodeprotonated L1, one fully deprotonated L2 ligand, and three coordinated water molecules. Both cobalt centers are six-coordinate, but their octahedral geometries display different coordination environments. The Co1 ion coordinates bidentately the phosphonate group of L2 and monodentately the phosphonate groups of three different L1 ligands, as well as one water molecule. On the other hand the Co2 ion coordinates one pyridyl N-atom and two phosphonate O-atoms from three different L2 ligands, one phosphonate O-atom of L1, as well as two water molecules. Each of the ligands L1 and L2 serves to link four metal centers (using two different coordination modes, $\eta^4\mu_4$ and $\eta^5\mu_4$, respectively) in order to form 2D MOF. Generally the 2D framework can be considered as formed from interweaved Co1–L1 and Co2–L2 ribbons (Figure 1). Using the topological analysis of Blatov and Proserpio the obtained network can be simplified as a 4-connected sql net presented with the Schläfli symbol $(4^4\cdot6^2)$ (Figure 2).¹

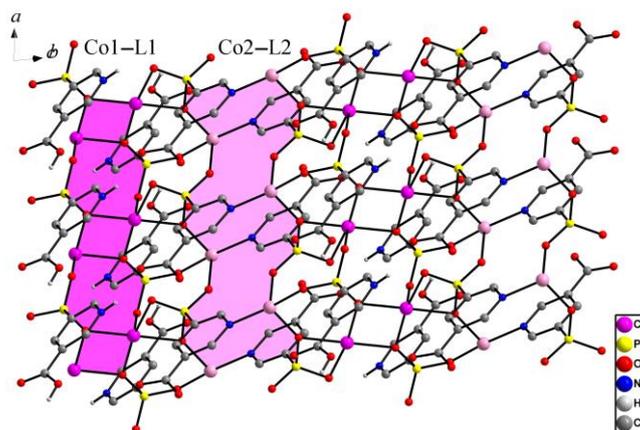


Figure 1. A view of the monolayer formed by interweaving Co1–L1 and Co2–L2 ribbons via Co–O(P) bonds. The terminal aqua ligands and the H atoms on the pyridine rings are omitted for clarity.

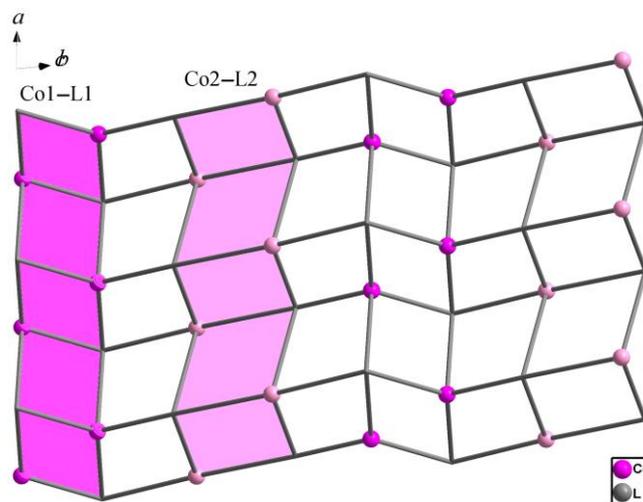


Figure 2. A schematic presentation of the 2D 4-connected sql net with $(4^4 \cdot 6^2)$ topology.

Reference

1. Blatov V. A. *IUCr CompComm Newsletter* **7**, 4 (2006).