Poster

# Crystal structure and computational study of cobalt(II) coordination polymer with 2,2'-dipyridylamine and anion of isophthalic acid

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Coordination polymers (CPs) utilizing the anions of benzenepolycarboxylic acids have received significant attention in crystal engineering due to the ability of these anions to form fascinating metal-organic crystal structures with various dimensionality and numerous applications as functional materials [1].

In our continual synthetic strategy of CPs [2-4], a new ongoing challenge was design and synthesis of ternary Co(II) complex with the anion of 1,3-benzenedicarboxylic acid (isophthalic acid, $H_2$ipht) and 2,2'-dipyridylamine (dipya). The single crystals of $[Co_6(dipya)_6(H_2O)(ipht)_6]_n$, **1**, have been solvothermally synthesized and characterized by single-crystal X-ray diffraction and computational analysis of noncovalent interactions. In **1**, there are six crystallographically different Co atoms: Co4 is in a deformed tetrahedral, Co2 is in an octahedral and Co1, Co3, Co5 and Co6 are in a square-pyramidal environment (Fig. 1). Each Co atom is coordinated by two bridging ipht ligands, which resulted in four different isotactic polymer zigzag chains running along *c*-axis: –Co5– mono/chelate ipht–Co6–monodentate/chelate ipht–Co5–, –Co4–bis-monodentate ipht–Co4–, –Co1–bis-chelate ipht–Co2–bis-monodentate ipht–Co1– and –Co3–monodentate/chelate ipht–Co3– (Fig. 1). The 3D supramolecular network is achieved through numerous noncovalent interactions. The Hirshfeld surfaces and corresponding 2D fingerprint plots of noncovalent interactions show that all types of close contacts are almost equally present in all four polymer chains. Further analysis based on surface properties suggests that the major stabilization in this supramolecular structure comes from the cooperation of stacking interactions between dipya ligands and N–H···O hydrogen bonds between dipya and ipht ligands, with important contributions of O–H···O hydrogen bonds between aqua and ipht ligands, as well as dipya/ipht and ipht/ipht aromatic C–H/π interactions.

*Crystal data*: $C_{108}H_{80}Co_6N_{18}O_{25}$, $M_r = 2383.5$, monoclinic system, space group $P2_1/c$, $a = 22.404(5)$, $b = 27.546(6)$, $c = 18.166(4)$ Å, $\beta = 111.71(3)$ °, $V = 10416(4)$ Å$^3$, $Z = 4$, $F(000) = 4864$, $\rho_x = 1.520$ g cm$^{-3}$, $\mu(\mathrm{Mo}\ K\alpha) = 1.018$ mm$^{-1}$. The refinement on $F^2$ (1420 parameters) yielded $R_1 = 0.0889$, $wR_2 = 0.1171$, $S = 1.02$ for all data, and $R_1 = 0.0491$ for 12629 observed reflections with $I \geq 2\sigma(I)$.

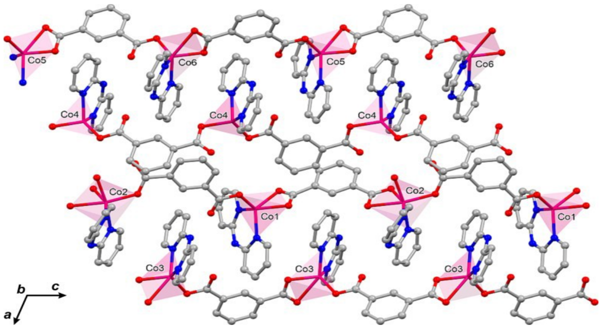

**Figure 1**. Polymeric chains of **1** running along *c*-axis.

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