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Encapsulation of one-dimensional cation chains into pseudo-channels by varying monomers with opposite charge

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ABSTRACT

Two compounds with cation chains and monomers, $[Co_{1/2}(bpbenz)_{1/2}]^{+}\cdot[Co_{1/2}(oba)]^{-}$ (**1**) and $[Ni(DPT)(H_2O)_4]^{2+}$ $[tpdc]^{2-}$ (**2**) have been synthesized under hydrothermal condition (bpbenz = 1,4-bis(4-pyridyl)benzene, H_2oba = 4,4′-oxybis- (benzoate), DPT = 2,5-dipyridinethiophene, H_2tpdc = biphenyldicarboxylic acid). In compound **1**, the monomer $[Co_{1/2}(oba)]^{-}$ anions stack in three orientations to generate a 1D pseudo channels encapsulation of cationic chains $[Co_{1/2}(bpbenz)_{1/2}]^{+}$. When considering the H-bonding interaction between coordinated water O atoms of the $[Co_{1/2}(bpbenz)_{1/2}]^{+}$ cationic chain and uncoordinated carboxylate oxygen atoms of the $[Co_{1/2}(oba)]^{-}$ anion, a binodal 3,6-coordinated 3D architecture is generated. Like **1**, the one-dimensional cation chains $[Ni(DPT)(H_2O)_4]^{2+}$ locate in pseudo-channels by $[tpdc]^{2-}$ monomers anions in compound **2**. A 3D net is also generated considering the H-bonding interaction.

Supramolecular architectures based on coordination compounds, where the metal centers are bridged by organic ligands, continue to be an interesting area of research [1–3]. In most cases, such compounds have some of the coordination sites occupied by coordinating organic ligands, whereas the remaining coordination sites are either empty or occupied by coordinating water ligand [4]. Over the past decade there has been a tremendous research interest in the construction of such materials mainly because of their intriguing architectures and novel physical properties that lead to potential applications in a series of areas including gas storage and separation [5,6], catalysis [7,8], opitics [9], magnetism [10], sensing [11,12]. However, in combination with appropriate ligands they can form compounds having either discrete (zero-dimensional, 0D), polyhedral, or infinite (one-, two-, and three-dimensional) structures [13]. The mixed ligands are undoubted good choice for construction of new nets. However, it is accompanied with even more uncertain elements. Therefore, the prediction of mixed-ligand architectures is still a challenge. Up to now, a number of N-donor bridging ligands have been widely employed to construct these coordination polymers. Herein, our synthetic strategy was to select bpbenz or DPT [14–16] and introduce V-shaped carboxylate ligands [17,18] into the reaction systems and construct two new coordination compounds with intriguing structures, that is, $[Co_{1/2}(bpbenz)_{1/2}]^{+}$ $[Co_{1/2}(oba)]^{-}$ (**1**) and $[Ni(DPT)(H_2O)_4]^{2+}$ $[tpdc]^{2-}$ (**2**): A mixture of $Co(NO_3)_2\cdot 6H_2O$ or $Ni(NO_3)_2\cdot 6H_2O$ (0.2 mmol), bpbenz or DPT (0.1 mmol) and H_2oba or H_2tpdc (0.2 mmol) was dissolved in 3 mL of distilled water and 3 mL of DMF. The final mixture was sealed in a 15 ml Parr Teflon-lined stainless-steel vessel and heated at 90 °C for 3 days, and then the reaction system was cooled to room temperature. Purple block crystals of **1** and green block crystals of **2** were obtained, respectively, washed with water, and dried under ambient conditions. (Yields: 58% for **1** based on bpbenz, 38% for **2** based on DPT). Elemental analysis (%) calcd for **1** ($H_{51}C_{53}N_5O_{15}Co_2$): C, 52.50; H, 4.41; N, 2.78. Found: C, 52.47; H, 4.46; N, 2.75. For **2**: ($C_{34}H_{28}N_2NiO_8S$): C, 59.76; H, 4.13; N, 4.10. Found: C, 59.69; H, 4.06; N, 4.01.

Compound **1** crystallizes in the triclinic space group *P*-1 [19]. Single-crystal X-ray diffraction studies reveal that the asymmetric units of **1** are composed of one $[Co_{1/2}(bpbenz)_{1/2}]^{+}$ cationic chain,

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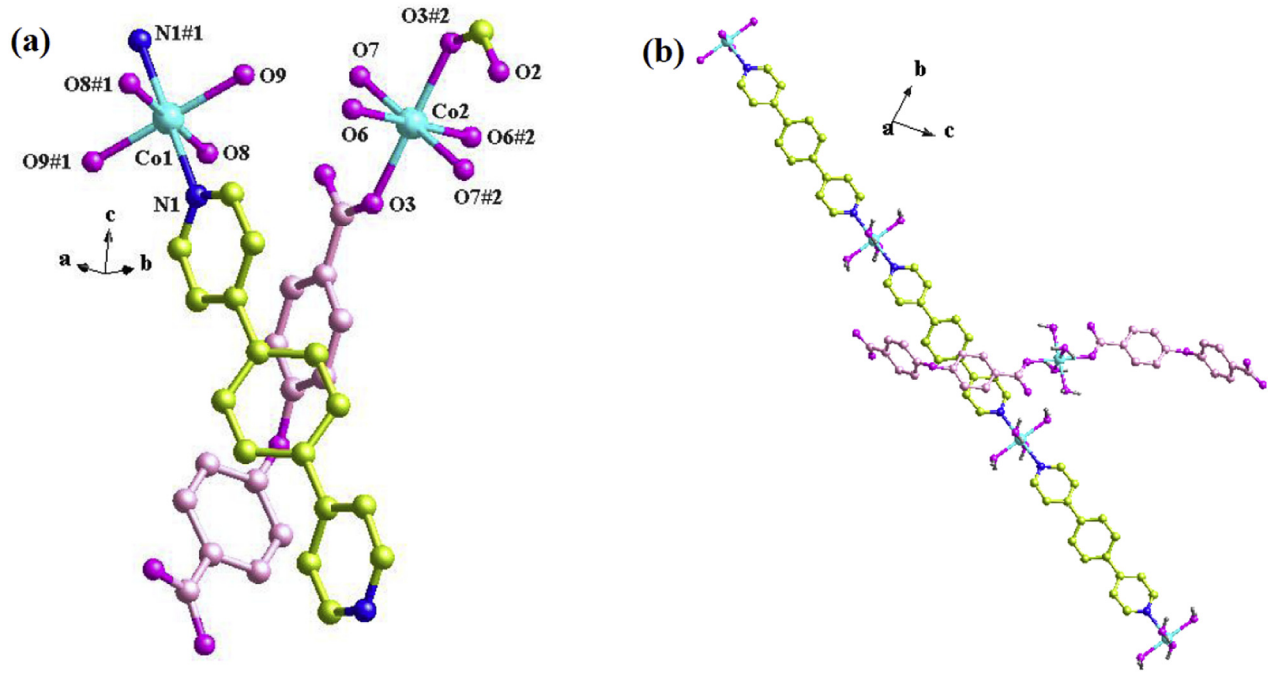

Fig. 1. (a) Coordination environment of the Co cation in **1**. The hydrogen atoms are omitted for clarity. Symmetry codes: #1 = 1 − *x*,−*y*, 1 − *z*; #2 = −*x*, 1 − *y*, 1 − *z*. (b) The structure contains $[Co_{1/2}(oba)]^-$ anion monomer and one-dimensional cationic chain $[Co_{1/2}(bpbenz)_{1/2}]^+_n$.

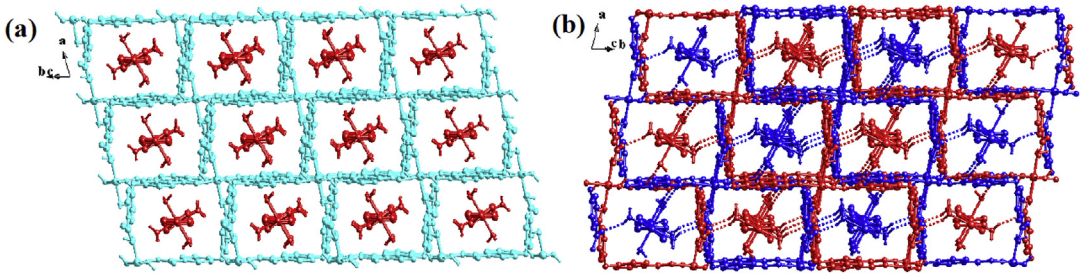

Fig. 2. (a) Encapsulation of one-dimensional cationic chains $[Co_{1/2}(bpbenz)_{1/2}]^+_n$ in pseudo channels formed by these $[Co_{1/2}(oba)]^-$ anions stacked in three orientations. (b) These hydrogen bonding interactions between coordinated H_2O molecule of $[Co_{1/2}(bpbenz)_{1/2}]^+$ cationic chain and carboxylate O atoms from $[Co_{1/2}(oba)]^-$ anions form a 2- fold interpenetrated framework.

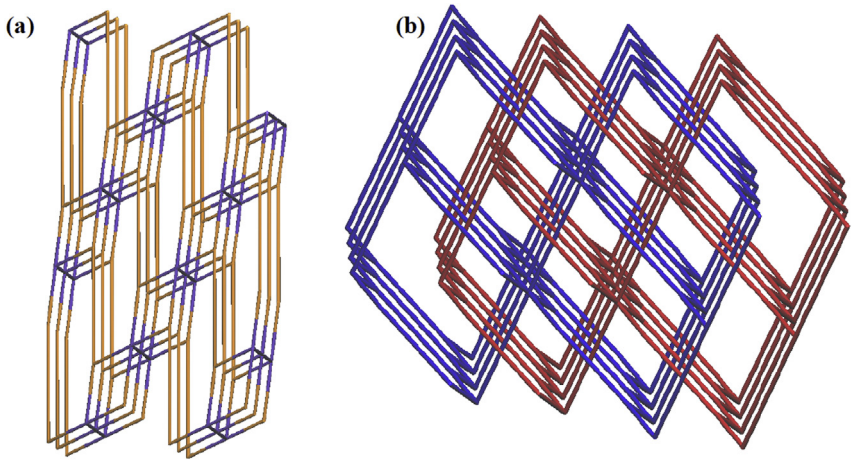

Fig. 3. (a) The binodal 3,6-coordinated 3D architecture with a *sqc27* topology considering the H-bond. (b) 2-fold interpenetrating 3D architecture **1**.