



NOTE

A New Mn(II) Coordination Polymer Based on Dicarboxylate and Imidazole-Containing Ligand

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A new coordination polymer with the composition $[\text{Mn}(\text{ada})(\text{bib})]_n \cdot 2\text{H}_2\text{O}$ (**1**) [H_2ada = 1,3-Adamantane dicarboxylic acid and bib = 4,4'-bis(imidazolyl)-biphenyl], has been prepared by hydrothermal synthesis. Complex $[\text{Mn}(\text{ada})(\text{bib})]_n \cdot 2\text{H}_2\text{O}$ (**1**), is Orthorhombic, space group $Pnma$ with $a = 14.352$ (5) Å, $b = 26.869$ (5) Å, $c = 11.576$ (5) Å, $V = 4464$ (3) Å³, $Z = 4$, $M_r = 904.89$, $D_c = 1.346$ g/cm³, $F(000) = 1896$ and $\mu = 0.357$ mm⁻¹. The final refinement gave $R = 0.0583$ and $wR = 0.0712$ for 2819 reflections with $I > 2\sigma(I)$. X-ray diffraction analysis reveals that complex **1** shows a two-dimensional (2D) layer structure.

Keywords: Coordination Polymer, Mn(II), Crystal Structure.

The design and synthesis of coordination frameworks represent a interesting active area, not only for their undisputed beauty with intriguing architectures and topologies but also for their potential applications as functional materials. It is well known that several factors, such as the metal centers, organic ligands, reaction temperatures, pH values and solvents have great influence in the final structures. Among these factors, the organic ligands play a crucial role in construction of coordination polymers. Polycarboxylic acids are frequently used for the construction of coordination polymers because of their variety of coordination modes and structural stability¹⁻⁶.

In this paper, we used 1,3-adamantane dicarboxylic acid (H_2ada) and 4,4'-bis(imidazolyl)biphenyl (bib) construct a new Mn(II) coordination polymer.

Materials and physical measurements: All reagents and solvents employed were commercially available and used without further purification. FT-IR spectra were recorded with a Bruker Equinox 55 FT-IR spectrometer as a dry KBr pellet in the 4000-400 cm⁻¹ range.

Preparation of $[\text{Mn}(\text{ada})(\text{bib})]_n \cdot 2\text{H}_2\text{O}$: The mixtures of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ (0.5 mmol), H_2ada (0.5 mmol), bib (0.5 mmol) and H_2O (12 mL) were sealed in a 25 mL Teflon-lined stainless steel vessel, the mixtures were heated at 120 °C for 96 h, and then cooled to room temperature. The yellow block crystals were obtained and washed with alcohol for several times (Yield: 37 % based on Mn). (KBr. ν_{max} , cm⁻¹): 3390 w, 1655 s, 1604 s, 1517 s, 1420 m, 1379 m, 1230 m, 1196 m, 1027 m, 967 m, 807 m.

X-ray crystallography: Single crystal X-ray diffraction analyses of complex **1** was carried out on a Bruker SMART APEXII CCD diffractometer equipped with a graphite monochromated $\text{MoK}\alpha$ radiation ($\lambda = 0.71073$ Å) by using a ω -scan mode. Empirical absorption correction was applied using the SADABS programs⁷. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHELX 97⁸. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement.

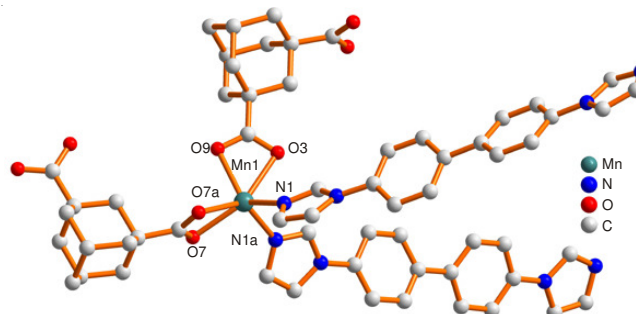


Fig. 1. Coordination environment of Mn(II) ion

Crystallographic analysis reveals that $[\text{Mn}(\text{ada})(\text{bib})]_n \cdot 2\text{H}_2\text{O}$ crystallized in the Orthorhombic, space group $Pnma$. The coordination environment around Mn(II) is shown in Fig. 1. The Mn(II) exhibits an octahedral geometry, with N_2O_4 coordina-

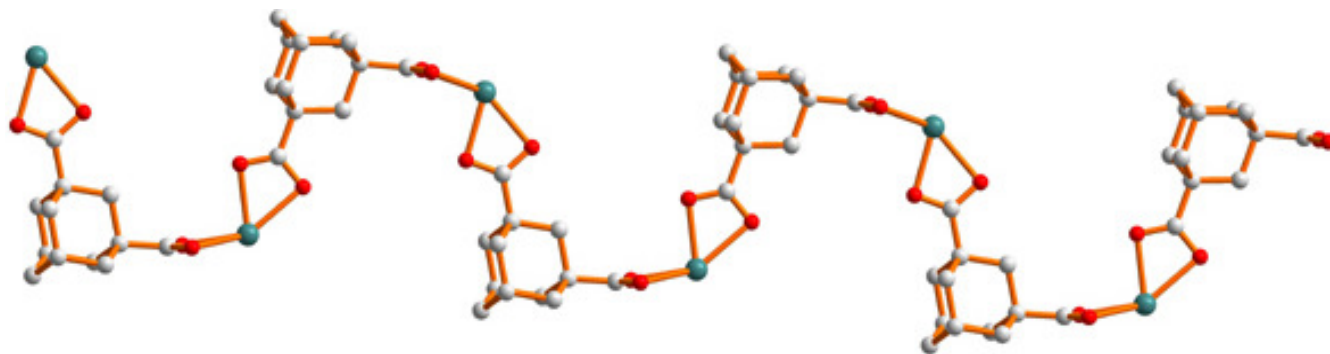


Fig. 2. 1D chain constructed by Mn(II) ions and carboxylate ligands

tion sphere from four carboxylate oxygen atoms [Mn-O, ranging from 2.220(5)-2.293(4) Å] and two nitrogen atoms [Mn(1)-N(1) = 2.167(3) Å]. The carboxylate ligands connect the Mn(II) ions to form a one-dimensional chain (Fig. 2). The 1D chains are further connected by bib ligands to construct a two-dimensional layer structure (Fig. 3).

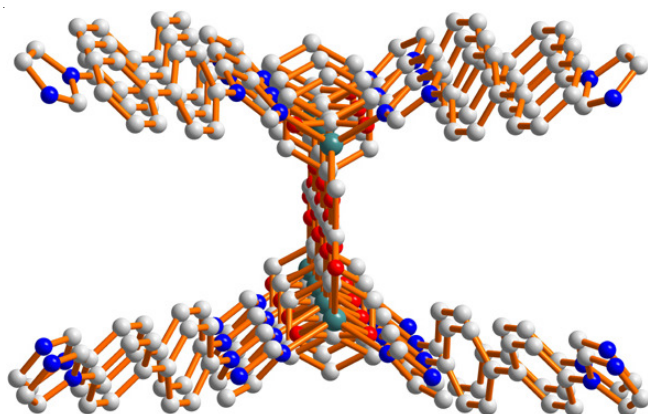


Fig. 3. 2D layer structure for complex 1

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