Synthesis, Crystal Structure and Theoretical Calculations of a Manganese(II) Coordination Polymer Assembled by 2,5-Thiophenedicarboxylic Acid and 3-(2-Pyridyl)pyrazole Ligands Postprint

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Abstract

A new Mn(II) complex, [Mn0.5(tdc)0.5(L)]2n (1, H2tdc = 2,5-thiophenedicarboxylic acid, L = 3-(2-pyridyl)pyrazole), has been successfully synthesized under hydrothermal conditions. Its structure has been determined by single-crystal X-ray diffraction analysis, elemental analyses, IR, TG and UV spectrum. Single-crystal X-ray diffraction analysis reveals that complex 1 belongs to the orthorhombic system, space group Pnna with a = 11.5184(6), b = 16.8399(8), c = 11.7249(5) Å, V = 2274.26(19) Å3, Z = 4, Dc = 1.505 g/cm3, = 0.715 mm-1, Mr = 515.41, F(000) = 1052, the final R = 0.0336 and wR = 0.0802 with I > 2 (I). It exhibits a one-dimensional zigzag-chain structure, which was stabilized through intermolecular C–H···O and intramolecular N–H···O hydrogen bonding interactions. Moreover, we analyzed Natural Bond Orbital (NBO) by using the PBE0/LANL2DZ method built in Gaussian 09 Program. The calculation results showed obvious covalent interaction between the coordinated atoms and Mn(II) ion.

Full Text

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ABSTRACT

A new Mn(II) complex, [Mn0.5(tdc)0.5(L)]2n (1, H2tdc = 2,5-thiophenedicarboxylic acid, L = 3-(2-pyridyl)pyrazole), has been successfully synthesized under hydrothermal conditions. Its structure has been determined by single-crystal X-ray diffraction analysis, elemental analyses, IR, TG and UV spectroscopy. Single-crystal X-ray diffraction analysis reveals that complex 1 belongs to the orthorhombic system, space group Pnna with a = 11.5184(6), b = 16.8399(8), c = 11.7249(5) Å, V = 2274.26(19) Å^3, Z = 4, Dc = 1.505 g/cm^3, = 0.715 mm^{1}, Mr = 515.41, F(000) = 1052, the final R = 0.0336 and wR = 0.0802 with I > 2 (I). It exhibits a one-dimensional zigzag-chain structure, which was stabilized through intermolecular C-H···O and intramolecular N-H···O hydrogen bonding interactions. Moreover, we analyzed Natural Bond Orbital (NBO) using the PBE0/LANL2DZ method built in Gaussian 09 Program. The calculation results showed obvious covalent interaction between the coordinated atoms and Mn(II) ion.

Keywords: hydrothermal synthesis; crystal structure; Mn(II) complex; natural bond orbital

1. INTRODUCTION

Recently, studies on the synthesis of coordination polymers (CPs) have gained considerable attention in coordination chemistry owing to their interesting molecular topologies and enormous potential applications in catalysis, molecular selection, non-linear optics, ion exchange and microelectronics [**?**]. Typically, the structural diversity of such crystalline materials depends on many factors, including counteranion, templating agents, metal ion, metal-ligand ratio, pH value, and the number of coordination sites provided by organic ligands [**?**]. In this context, the judicious selection of organic ligands or coligands based on their length, rigidity, and functional groups is important for the assembly of structurally controllable CPs, and many significant studies have been conducted using this strategy [**?**]. Usually, organic ligands with bent backbones, such as V-shaped, triangular, quadrangular, and similar architectures, are excellent candidates for building highly connected, interpenetrating, or helical coordination structures due to their bent backbones and versatile bridging fashions [?, ?]. Moreover, carboxylate groups serve as good hydrogen-bond acceptors as well as donors, depending on the degree of deprotonation. Among these, quadrangular polycarboxylic acids, such as 1,2,4,5-benzenetetracarboxylic acid, 3,3 ,4,4 -benzophenone tetracarboxylic acid, 4,4 -oxydibenzoic acid and 2,5-thiophenedicarboxylic acid, have received much attention owing to their rich coordination modes [?]. Apart from the carboxylate linkers, chelating N-donor ligands, such as 1,10-phenanthroline, 2,2 -bipyridine, and 3-(2-pyridyl)pyrazole, are frequently used in the assembly process of CPs [?].

These considerations motivated us to investigate new coordination frameworks with 2,5-thiophenedicarboxylic acid (H2tdc) and an N-donor ligand (L). Here, we report the synthesis and characterization of a new CP, namely [Mn0.5(tdc)0.5(L)]2n (1), which exhibits a one-dimensional zigzag-chain structure that is distinct from those of previously reported 2,5-thiophenedicarboxylate-bridged complexes [?].

2. EXPERIMENTAL

2.1 General Procedures

All chemicals were purchased commercially and used without further purification. Elemental analyses (C, H and N) were measured on a Perkin-Elmer 2400 CHN Elemental Analyzer. IR spectra were recorded in the range of 4000–400 cm 1 on a Nicolet 6700 Spectrophotometer using KBr pellets. TG studies were carried out on a STA7300 analyzer under nitrogen at a heating rate of 10 ℃・min 1. Powder X-ray diffraction (PXRD) patterns were collected in the 2 range of 5–50° with a scan speed of 0.1°・s 1 on a Bruker D8 Advance instrument using CuK radiation (= 1.54056 Å) at room temperature. UV spectra were obtained on a Shimadzu UV-250 spectrometer in the 200–400 nm range.

2.2 Synthesis of [Mn0.5(tdc)0.5(L)]2n (1)

A mixture of Mn(OAc) ・4H O (0.05 g, 0.2 mmol), H tdc (0.068 g, 0.4 mmol), and L (0.029 g, 0.2 mmol) was dissolved in 18 mL H O. The final mixture was placed in a Parr Teflon-lined stainless-steel vessel (30 mL) under autogenous pressure and heated at 150 ℃ for five days, yielding block crystals. The reaction yield was approximately 42%. Anal. Calcd. for C H MnN O S: C, 51.27; H, 3.13; N, 16.31%. Found: C, 50.01; H, 2.85; N, 16.03%. IR (cm 1): 3113(w), 3023(w), 1944(w), 1604(s), 1582(m), 1533(m), 1432(m), 1360(s), 1306(w), 1250(w), 1229(m), 1154(w), 1114(w), 1111(w), 1094(w), 1065(w), 1015(w), 963(m), 899(w), 839(w), 792(s), 766(s), 709(w), 698(w), 682(w), 633(w), 593(w), 486(m), 469(w).

2.3 X-ray Crystallography

All diffraction data for complex 1 were collected on a Bruker/Siemens Smart Apex II CCD diffractometer with graphite-monochromated MoK radiation (= 0.71073 Å) at 293(2) K. Data reductions and absorption corrections were performed using the SAINT and SADABS programs, respectively. The structures were solved by direct methods, and all non-hydrogen atoms were refined anisotropically on F^2 by full-matrix least-squares technique using the SHELXL-97 crystallographic software package [?, ?]. All hydrogen atoms were generated geometrically and refined isotropically using the riding model. For 1, a total of 2818 reflections were collected in the range of 3.74 28.38°, of which 2368 were independent (Rint = 0.0306). The final R = 0.0295 and wR = 0.1030 for the observed reflections with I > 2 (I), and R = 0.0336 and wR = 0.0802 for all data with (Δ)max = 0.289 and (Δ)min = -0.332 e · Å ^{3}. Selected bond lengths and bond angles of complex 1 are shown in Table 1 . Hydrogen bonding geometry for the title complex is collected in Table 2 .

2.4 Theoretical Calculations

All calculations in this work were performed using the Gaussian09 program [?]. The molecular structure parameters for calculation were all taken from the experimental data of the complex. Natural bond orbital (NBO) analysis was carried out by density functional theory (DFT) [?] with the PBE0 [?] hybrid functional and the LANL2DZ basis set [?].

3. RESULTS AND DISCUSSION

3.1 IR Spectrum

The IR spectrum of 1 shows a broad absorption band at 3023 cm ^{1} corresponding to C–H stretching. Asymmetric and symmetric COO stretching modes of the lattice tdc^{2} anion were evidenced by very strong, slightly broadened bands at 1604 and 1360 cm ^{1} [?], which is consistent with the results of X-ray analysis.

3.2 Structure Description

Single-crystal X-ray diffraction analysis reveals that complex 1 crystallizes in the orthorhombic space group Pnna and exhibits a one-dimensional zigzag-chain structure. The coordination environment of Mn(II) in 1 is shown in Fig. 1 [Figure 1: see original paper]. There are half a Mn(II) ion, half a tdc ligand and one L ligand in the asymmetric unit. The Mn(1) ion is six-coordinated by two carboxylate oxygen atoms (O(1), O(1A)) from two different tdc ligands and four nitrogen donors (N(2), N(2A), N(3), N(3A)) from two L molecules to form a distorted octahedral coordination geometry. The Mn–O bond distances in compound 1 are 2.1322(12) Å, and the Mn–N bond lengths fall in the range of 2.1915(14)-2.4086(15) Å, which are within normal ranges, and the coordination angles around the Mn atom vary from 70.43(5) to 166.75(5)° [?]. In the coordination environment, one carboxylate oxygen atom (O(1)) and three nitrogen atoms (N(2), N(2A), N(3)) lie in the basal plane, while one carboxylate oxygen atom (O(1A)) and nitrogen atom (N(3A)) occupy the axial positions from opposite directions. One coordination mode of the tdc ligand is present in the structure of complex 1, namely a monodentate bridging mode. The L ligand exhibits a chelating mode, through which two Mn(II) ions are linked by tdc ligands to produce a one-dimensional zigzag chain, which differs from previously reported 2,5-thiophenedicarboxylate-bridged complexes [?]. The distance between neighboring Mn(II) ions is approximately 11.331 Å, as illustrated in Fig. 2 [Figure 2: see original paper]. The L ligands are located above and below the chain.

Hydrogen bonding interactions are frequently important in the synthesis of supramolecular frameworks. There are persistent intermolecular C–H···O and intramolecular N–H···N hydrogen bonding interactions between carboxylate oxygen atoms of tdc ligands, nitrogen atoms and carbon atoms of L ligands in complex 1 (Table 2). Thus, through hydrogen bonds, the one-dimensional zigzag chains are further expanded into a three-dimensional supramolecular architecture (Fig. 3 [Figure 3: see original paper]), which plays an important role in stabilizing complex 1.

3.3 Powder X-ray Diffraction (PXRD) and Thermal Stability

To confirm the phase purity of complex 1, powder X-ray diffraction patterns were recorded and found to be comparable to the corresponding simulated patterns calculated from single-crystal diffraction data (Fig. 4 [Figure 4: see original paper]), indicating a pure phase of the bulk sample.

The TG curve of 1 (Fig. 5 [Figure 5: see original paper]) shows that the first weight loss of 34.2% from 317 to 400 ℃ corresponds to the removal of the tdc ligand (calcd: 33.0%). Upon further heating, a clear weight loss (54.8%) occurs in the temperature range of 400–710 ℃, corresponding to the release of the L ligand (calcd: 56.3%). After 710 ℃, no further weight loss is observed, indicating complete decomposition of 1; the residual weight should be MnO.

3.4 UV Spectrum Analysis

The UV spectra for complex 1, H tdc and L ligands have been recorded in the solid state. H tdc has one absorption band at approximately 273 nm and L has one absorption band at approximately 280 nm, whereas the title complex 1 has one absorption band at approximately 281 nm (Fig. 6 [Figure 6: see original paper]), which should be assigned to the n→ * transition of the ligands and the charge transfer transition [?].

4. THEORETICAL CALCULATIONS

The selected natural atomic charges and natural electron configurations for the complex are displayed in Table 3 . The results show that the electronic configurations of the Mn(II) ion, N and O atoms are 4s $\cdot^{22}$3d $\cdot$ ^{1}4p $\cdot^{3}$, 2s$^{1}\cdot^{32}$–$^{1}\cdot^{33}$2p $\cdot$ ^{12}– $\cdot^{13}$ and 2s$^{1}\cdot$ 2p $\cdot$ ^{3}, respectively. Based on these results, one can infer that the coordination of the Mn(II) ion with N and O atoms involves primarily the 3d, 4s, and 4p orbitals. N atoms form coordination bonds with the Mn(II) ion using 2s and 2p orbitals. All O atoms donate electrons from 2s and 2p orbitals to the Mn(II) ion to form coordination bonds. Thus, the Mn(II) ion receives electron density from four N atoms of L and two O atoms of tdc [?]. Therefore, on the basis of valence-bond theory, the atomic net charge distribution and NBO bond orders of 1 (Table 3) indicate obvious covalent interaction between the coordinated atoms and the Mn(II) ion. The differences in NBO bond orders for Mn–O and Mn–N bonds account for their different bond lengths [?], which is in good agreement with the X-ray crystal structural data of compound 1.

As can be seen from Fig. 7 [Figure 7: see original paper], the lowest unoccupied molecular orbital (LUMO) consists mainly of the L ligand, whereas the highest occupied molecular orbital (HOMO) is composed primarily of the metal center. Thus, charge transfer from metal to ligand may be deduced from the molecular orbital contours of complex 1.

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Table 1. Selected Bond Lengths (Å) and Bond Angles (°) for Complex 1

Distances		Angles	
Mn(1)-O(1)	2.1322(12)	O(1)-Mn(1)-O(1A)	95.55(7)
Mn(1)-O(1A)	2.1322(12)	O(1)-Mn(1)-N(2)	101.92(5)
Mn(1)-N(2)	2.1915(14)	O(1)-Mn(1)-N(2A)	97.73(5)
Mn(1)-N(2A)	2.1915(14)	O(1)-Mn(1)-N(3A)	166.75(5)
Mn(1)-N(3)	2.4086(15)	O(1A)-Mn(1)-N(2)	97.73(5)
Mn(1)-N(3A)	2.4086(15)	O(1A)-Mn(1)-N(2A)	101.92(5)
		O(1A)-Mn(1)-N(3)	166.75(5)
		O(1A)-Mn(1)-N(3A)	92.81(5)
		N(2)-Mn(1)-N(2A)	150.61(8)
		N(2)-Mn(1)-N(3A)	70.43(5)
		N(2A)-Mn(1)-N(3A)	87.08(5)

Symmetry transformations used to generate equivalent atoms: A: -x, -y, -z

Table 2. Hydrogen Bonds for Complex 1

Table 3. Natural Atomic Charges, Natural Valence Electron Configurations, Wiberg Bond Indexes and NBO Bond Orders (a.u.) for Complex 1

Atom/Interaction	Natural Charge	Electron Configuration	Wiberg Bond Index	NBO Bond Order
Mn(1)		[core]4s(0.22)3d(5.51)4p(0.39)		
O(1)		[core]2s(1.65)2p(5.03)		
O(1A)		[core]2s(1.65)2p(5.03)		
N(2)		[core]2s(1.33)2p(3.93)		
N(2A)		[core]2s(1.33)2p(3.93)		
N(3)		[core]2s(1.32)2p(4.11)		
N(3A)		[core]2s(1.32)2p(4.11)		
Mn(1)-O(1)				
Mn(1)-O(1A)				
Mn(1)-N(2)				

Atom/Interaction	Natural Charge	Electron Configuration	Wiberg Bond Index	NBO Bond Order
Mn(1)-N(2A)				
Mn(1)-N(3)				
Mn(1)-N(3A)				

Figure 1. Coordination environment of the Mn(II) center in 1. Symmetry code: (A) -x, -y, -z

Figure 2. View of the one-dimensional zigzag chain

Figure 3. View of the 3D supramolecular architecture of 1 formed by hydrogen-bonding interactions

Figure 4. PXRD analysis of the title complex: bottom—simulated, top—experimental

Figure 5. TGA curve of complex 1

Figure 6. UV spectrum of 1 at room temperature

Figure 7. Frontier molecular orbitals of complex 1

Note: Figure translations are in progress. See original paper for figures.

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