Syntheses, Crystal Structures and Characterization of Two Coordination Polymers Based on Mixed Ligands (Post-print)

Authors: WANG Yu-Fang, HE Chao-Jun

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Abstract

Two new coordination polymers, namely, {[Cd1.5(bc)2(HL)].H2O}2n (1) and [Mn(ip)(H2L)(H2O)]n (2) (H2L = 3-(1H-pyrazol-4-yl)-5-(pyridin-2-yl)-1,2,4-triazole, Hbc = benzoic acid, H2ip = isophthalic acid) were constructed by solvothermal reaction. The compounds were characterized by elemental analysis, FT-IR spectroscopy, and single-crystal X-ray diffraction. Compound 1 displays a two-dimensional plane structure consisting of [Cd3(bc)2(HL)] subunits. Compound 2 possesses a one-dimensional chain structure and is further extended into a 3-D supramolecular architecture via hydrogen bonds. Moreover, photoluminescence studies showed compound 1 exhibits luminescent emissions with emission maxima at 375 nm. Magnetic susceptibility measurements of 2 indicate that domain antiferromagnetic interactions exist between Mn(II) ions. In addition, thermogravimetric properties of 1 and 2 were also measured.

Full Text

Preamble

Syntheses, Crystal Structures and Characterization of Two Coordination Polymers Based on Mixed Ligands

Yu-Fang Wang (1), **Chao-Jun He** (2)
(1) College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-oriented Porous Materials, Luoyang Normal University, Luoyang 471934, China
(2) School of Food and Drug, Luoyang Normal University, Luoyang, Henan 471934, China

ABSTRACT

Two new coordination polymers, namely {[Cd . (bc) (HL)] • H O} (1) and [Mn(ip)(H L)(H O)] (2) (H L = 3-(1H-pyrazol-4-yl)-5-(pyridin-2-yl)-1,2,4-triazole, Hbc = benzoic acid, H ip = isophthalic acid), were constructed by solvothermal reaction. The compounds were characterized by elemental analysis, FT-IR spectroscopy, and single-crystal X-ray diffraction. Compound 1 displays a two-dimensional layered structure consisting of [Cd (bc) (HL)] subunits. Compound 2 possesses a one-dimensional chain structure and is further extended into a 3-D supramolecular architecture via hydrogen bonds. Moreover, photoluminescence studies showed that compound 1 exhibits luminescent emissions with emission maxima at 375 nm. Magnetic susceptibility measurements of 2 indicate that weak antiferromagnetic interactions exist between Mn(II) ions. In addition, thermogravimetric properties of 1 and 2 were also measured.

Keywords: cadmium(II); manganese(II); crystal structure; luminescence; magnetic property
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1 INTRODUCTION

The design and synthesis of new coordination polymers are nowadays a challenging research topic that attracts increasing interest due to the creation of various intriguing architectures and their potential applications of such metal-organic materials. As we all know, the selection of organic ligands is very important in the construction of coordination polymers. Recently, N-donor ligands have been widely employed in the construction of coordination polymers or metal-organic frameworks with intriguing structure. To modulate the structure, different polycarboxylate ligands can be used as auxiliary ligands to direct the self-assembly. Although the appealing topology and interesting properties of metal coordination frameworks that have been synthesized by various N-donor ligands and aromatic carboxylic acid have so far been explored to a great extent in the area of crystal engineering to date, the synthesis of compositionally and structurally designed MOFs and their composites remains a significant challenge nowadays owing to the difficulty in fine-tuning the phase distributions and architectures of final products. We selected 3-(1H-pyrazol-4-yl)-5-(pyridin-2-yl)-1,2,4-triazole as ligand and benzoic and isophthalic acids as auxiliary ligands in this paper. Herein we synthesized two new coordination polymers, {[Cd . (bc) (HL)] • H O} (1) and [Mn(ip)(H L)(H O)] (2). Their structure-induced physical properties, thermal stability, photoluminescence, magnetic properties, and so forth are also described and discussed.

2 EXPERIMENTAL

2.1 Materials and Characterization

All reagents were of analytical grade and used without further purification. Elemental analyses for carbon, hydrogen, and nitrogen atoms were carried out on a Vario EL III elemental analyzer. The IR spectrum was recorded (400–4000 cm ^{1} region) on a SHIMADZU IR Affinity-1S Spectrometer. All fluorescence measurements were carried out on an F-7000 Fluorescence Spectrophotometer (220–240V). Thermogravimetric analyses (TGA) were carried out in nitrogen at a heating rate of 10 °C · min ^{1} using a TG/DTA 6300 integration thermal analyzer. Variable-temperature magnetic susceptibilities were measured on a MPMS-7 SQUID magnetometer. Diamagnetic corrections were made with Pascal' s constants for all constituent atoms.

2.2 Preparation of {[Cd . (bc) (HL)] · H O} (1)

A mixture of Cd(NO) · 4H O (92.5 mg, 0.30 mmol), H L (21.2 mg, 0.10 mmol), Hbc (36.6 mg, 0.30 mmol), and KOH (11.2 mg, 0.2 mmol) was dissolved in H O, added to a 10 mL small glass bottle after stirring, and then sealed in a 25 mL Teflon-lined stainless-steel autoclave at 130 °C for 72 h, followed by slowly cooling to room temperature at a rate of 5 °C · h ^{1}. Light yellow block-shaped crystals were obtained in 54% yield, washed with water, and air-dried. IR (cm ^{1}): 3433(w), 3180(w), 2976(w), 2363(m), 2336(m), 1581(m), 1536(m), 1526(m), 1383(m), 1300(m), 1150(m), 1069(m), 1025(m), 952(m), 848(m), 765(m), 710(m), 670(m), 518(m), 473(m). Anal. Calcd. (%) for C H Cd . N O : C, 45.03; H, 2.99; N, 13.13. Found (%): C, 45.55; H, 2.92; N, 13.10.

2.3 Preparation of [Mn(ip)(H L)(H O)] (2)

The preparation of 2 was similar to that of 1 except that MnSO · 4H O and Hbc were used instead of Cd(NO) · 4H O and H ip. Light-brown crystals of 2 were obtained in 50% yield. IR (cm ^{1}): 3429(w), 3056(w), 2465(m), 2320(m), 1617(m), 1595(m), 1558(m), 1476(m), 1401(m), 1308(m), 1196(m), 1057(m), 784(m), 716(m). Anal. Calcd. (%) for C H MnN O : C, 48.12; H, 3.14; N, 18.71. Found (%): C, 48.45; H, 3.12; N, 18.58.

2.4 Crystal Structure Determination

Single-crystal X-ray diffraction data of compounds 1 and 2 were collected with a Rigaku Oxford SuperNova diffractometer with MoK radiation (= 0.71073 Å). Intensities were collected and reduced using the program CrysAlisPro (Rigaku Oxford, Version 1.171.39.3a), and a multi-scan absorption correction was applied. The structures were solved by direct methods with SHELXS-97 and refined on F^2 by full-matrix least-squares with SHELXL-97. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were assigned with common isotropic displacement factors and included in the final refinement using geometrical restraints. The details of crystal parameters are summarized in Table 1 , and the selected bond lengths are listed in Table 2 .

3 RESULTS AND DISCUSSION

3.1 Structure Description

3.1.1 Crystal Structure of {[Cd . (bc) (HL)] · H O} (1) Compound 1 crystallizes in the monoclinic space group P2 /n and exhibits a 2D layered framework. Its asymmetric unit contains one and a half Cd atoms, one HL ligand, two bc ligands, and one uncoordinated water molecule. As shown in Fig. 1 [Figure 1: see original paper], the two Cd(II) ions in 1 are both six-coordinated. The Cd(1) ion with 1/2 occupation is coordinated by two nitrogen atoms (N(4), N(4)#1) of two different H L ligands and four oxygen atoms (O(2), O(2)#1, O(3), O(3)#1) from four different Hbc ligands. The Cd(1) is located at an inversion center. Cd(2) is coordinated by three nitrogen atoms (N(1), N(3), N(6)#2) of two different H L ligands and three oxygen atoms (O(1), O(3), and O(4)) from two different bc ligands. Two adjacent Cd(II) atoms are bridged by O(1) and O(2) atoms of the carboxylate group from one bc ligand and a bifurcated O(3) atom of the carboxylate group from another bc ligand, while another O(4) atom of the carboxylate group from this bc ligand is linked to the Cd(2) atom. Simultaneously, the two adjacent Cd(II) ions are bridged by N(3) and N(4) atoms of triazole from the HL ligand, and the N(1) atom of pyridine from this HL ligand is linked to the Cd(2) ion. The Cd–O distances fall in the range of 2.1892(19)-2.5890(19) Å, and the Cd–N distances vary from 2.261(2) to 2.403(2) Å. These bond angles and bond distances all fall within normal ranges. In compound 1, two pairs of oppositely arranged bc anions and one pair of oppositely arranged HL anions bind three Cd(II) ions (two Cd(2) and one Cd(1)) to form the [Cd (bc) (HL)] subunit, with the Cd(1) ··· Cd(2) separation of 3.806 Å. The trinuclear subunits are then linked to form an infinite two-dimensional network through an HL ligand bridging mode (Fig. 2 [Figure 2: see original paper]).

In the crystal packing, hydrogen bonding interactions exist among uncoordinated water molecules and nitrogen atoms of HL ligands and oxygen atoms of bc ligands: N(5)-H(5) ··· O(5)#1 (H ··· O/N ··· O distance = 1.96/2.749(3) Å, angle = 152.3°); O(5)-H(5A) · · · N(2)#2 (H · · · N/O · · · N distance = 1.94/2.789(3) Å, angle = 171.9°); O(5)-H(5B) ··· O(4) (H ··· O/O ··· O distance = 1.94/2.738(3) Å, angle = 157.2°). The 2D architecture of 1 is also reinforced by extensive hydrogen bonding interactions.

3.1.2 Crystal Structure of [Mn(ip)(H L)(H O)] (2) X-ray single-crystal diffraction analysis reveals that 2 crystallizes in the monoclinic system, space group P2 /n, and exhibits a 1D framework. As shown in Fig. 3 [Figure 3: see original paper], the asymmetric unit contains one Mn(II) ion, one H L ligand, and one ip^{2} ligand. The Mn(II) center is five-coordinated to two nitrogen atoms (N(2) and N(3)) from the same H L ligand, three oxygen atoms (O(1), O(4)#1) from two different H ip ligands, and one oxygen atom (O(5)) from one coordinated water molecule. The Mn–N distances are 2.223(2) and 2.260(2) Å, respectively, and the Mn–O lengths fall in the range of 2.1653(18)–2.2175(18) Å, which are within the normal range observed in manganese complexes. Weak coordination bonds exist in 2 (Mn(1) ··· O(2) = 2.665 Å and Mn(1) ··· O(3) = 2.559 Å), resulting in two carboxylate groups of the ip^{2} ligand being nearly coplanar. The H L ligand adopts a chelating mode to connect one Mn(II) atom through one imidazole N atom and one pyridine N atom. Meanwhile, two carboxyl groups of the ip^{2} ligand in compound 2 are completely deprotonated and exhibit a -^{1}:^{1} coordination mode to link two Mn(II) ions, finally forming a one-dimensional chain with Mn ··· Mn distances of 10.160 Å.

In the crystal packing, H-bonding interactions exist among the pyridine N atom, imidazole N atom, coordinated water molecule, and carboxyl groups of the ip^{2} ligand: N(5)–H(5) ··· O(2) (H ··· O/N ··· O distance = 1.995/2.831 Å, angle = 163.6°); O(5)–H(5A) ··· O(1) (H ··· N/O ··· O distance = 1.865/2.747 Å, angle = 153.8°); O(5)–H(5B) ··· O(4) (H ··· N/O ··· O distance = 1.933/2.756 Å, angle = 162.5°); N(7)–H(7) ··· O(3) (H ··· N/N ··· O distance = 2.268/2.918 Å, angle = 132.5°). In addition, ··· stacking interactions exist between the nearest neighboring benzene rings which are parallel to each other with interplane distances of 4.070 Å. These hydrogen bonds and ··· stacking interactions lead to the formation of a 3-D supramolecular network (Fig. 4 [Figure 4: see original paper]), in which the Mn ··· Mn separation is 4.800 Å.

3.2 Luminescence Spectra of Compound 1

As shown in Fig. 5 [Figure 5: see original paper], complexes with d^{1} metal centers have been investigated for fluorescent properties and potential applications as fluorescence-emitting materials. It should be noted that the H L ligand displays fluorescence in the solid state at room temperature, while compound 1 exhibits different fluorescence. The ligand maximum appears at an excitation wavelength = 325 nm, with a maximum emission peak at = 380 nm. In compound 1, there is an excitation maximum at 270 nm with a maximum emission peak at 375 nm. Compared with the ligand H L, the emission peak of compound 1 shows a slight blue shift from 380 to 375 nm. This phenomenon is best ascribed to metal-to-ligand charge transfer according to the literature.

3.3 Magnetic Properties of Compound 2

For compound 2, the solid-state magnetic susceptibility was measured on a polycrystalline sample at 2000 Oe over the temperature range of 2–300 K. A plot of the T vs. T susceptibility data for 2 is shown in Fig. 6 [Figure 6: see original paper]. The value of T at 300 K is 8.80 emu mol ^{1} K, which is slightly higher than the expected spin-only value for two Mn(II) ions (8.75 emu mol ^{1} K). As the temperature is lowered, the T value decreases slowly to 8.75 emu mol ^{1} K at 2 K, indicating the presence of weak antiferromagnetic interactions within the sample.

The crystal packing of 2, which is driven by hydrogen-bonding, reveals an intermolecular Mn···Mn separation distance of 4.800 Å, compared to the intrachain Mn···Mn separation distance of 10.160 Å. The Mn–Mn dinuclear fragment formed by the two Mn-COO···HO(H)–Mn paths is characterized by the shortest metal-metal separation distance (4.800 Å). Moreover, magnetic exchange between transition metal centers through hydrogen-bonding interactions involving coordinated water molecules is well-documented in the literature. The Heisenberg spin Hamiltonian model ($\hat{H}$ = -JS S , S = S = 5/2) for the isotropic magnetic exchange interaction in the dinuclear Mn(2) unit is given in Eq. (1).

$$\frac{Ng^2\beta^2}{kT}\cdot\frac{A}{B}$$

where

$$A = 55\exp[30J/kT]+30\exp[20J/kT]+14\exp[12J/kT]+5\exp[6J/kT]+\exp[2J/kT]$$

$$B = 1+11\exp[30J/kT]+9\exp[20J/kT]+7\exp[12J/kT]+5\exp[6J/kT]+3\exp[2J/kT]$$

A good fit was achieved with the fitting parameters as follows: J = -0.23 cm ^{1}, g = 2.004, and the agreement factor R = Σ[( ) b -( )ca c]^{2}/Σ( )^{2} b is 1.08 × 10 . The analysis confirms weak antiferromagnetic interactions between the Mn(II) atoms bridged by hydrogen-bonding. The hydrogen interactions provide an effective pathway for magnetic exchange between Mn(II) atoms. The small J value observed may be explained by the fact that the magnetic orbitals are unfavorably oriented to interact.

3.4 Thermogravimetric Analyses of Compounds 1 and 2

To further characterize compounds 1 and 2, their thermal analyses were performed under N atmosphere at a heating rate of 10 °C/min in the temperature range of 30–800 °C. As shown in Fig. 7 [Figure 7: see original paper], the TGA curves of 1 and 2 indicate that the samples undergo two main weight loss steps, with coordinated water molecules being lost in the ranges of 140–190 °C and 160–240 °C for 1 and 2, respectively. The weight losses of 2.92% and 4.18% are consistent with the calculated values (2.81% and 4.01%). The frameworks then begin to decompose with continuous weight loss above 260 °C and 340 °C for 1 and 2, respectively. The final residues of 29.63% (calcd. 30.06%) for 1 and 15.58% (calcd. 15.78%) for 2 may be CdO and MnO powder, respectively.

These results suggest that the backbone of 2 is more thermally robust than that of 1 and can resist decomposition at temperatures up to 340 °C.

3.5 XRD Analyses

To verify whether the crystal structures are truly representative of the bulk materials, powder X-ray diffraction (PXRD) experiments were carried out for 1 and 2 at room temperature. As shown in Fig. 8 [Figure 8: see original paper], the peak positions of the simulated and experimental PXRD patterns are in agreement with each other, demonstrating that the bulk synthesized materials and the measured single crystals are identical.

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Fig. 1. Coordination environment of Cd(II) ions in 1
Fig. 2. 2D network structure of 1
Fig. 3. Coordination environment of the Mn(II) ion in 2
Fig. 4. 3D supramolecular structure of 2
Fig. 5. Emission spectra for 1 in the solid state
Fig. 6. Temperature dependence of T ( ) and ( ) for 2 and their corresponding theoretical curves (solid lines)
Fig. 7. TGA curves of compounds 1 and 2
Fig. 8. PXRD patterns of compounds 1 and 2

Table 1. Crystal Data and Details of Experiment for Compounds 1 and 2

Parameter	Compound 1	Compound 2
Empirical formula	C H Cd . N O	C H MnN O
Formula weight	-	-
Temperature (K)	293(2)	293(2)
Crystal system	Monoclinic	Monoclinic
Space group	P2 /n	P2 /n
Cell parameters (Å, °)	a = 12.1665(3), = 90b = 11.4872(2), = 93.157(2)c = 17.2589(4), = 90	a = 9.0415(5), = 90b = 22.0030(11), = 112.969(7)c = 10.1605(7), = 90
Volume (Å^3)	2408.43(9)	1861.1(2)
Calculated density (g/cm^3)	-	-
Absorption coefficient (mm^{1})	-	-
F(000)	-	-
Crystal size (mm^3)	0.20 × 0.20 × 0.18	0.18 × 0.18 × 0.20
2 range for data collection (°)	6.666–51	7.06–51.998
Index ranges	-14 h 14-13 k 13-20 l 20	-11 h 12-27 k 27-13 l 12
Reflections collected	-	-
Independent reflections	4425 (R = 0.0296)	3648 (R = 0.0475)
Data/restraints/parameters	4425/0/334	3648/0/272
Goodness-of-fit on F^2	-	-
Final R indexes (I > 2 (I))	R = 0.0277, wR = 0.0548	R = 0.0445, wR = 0.0969
Final R indexes (all data)	R = 0.0337, wR = 0.0577	R = 0.0602, wR = 0.1027
Largest diff. peak and hole (e • Å^3)	0.35 and -0.37	0.35/-0.35

Table 2. Selected Bond Lengths (Å) and Bond Angles (°) of Compounds 1 and 2

Compound 1: - Cd(1)-O(2)#1: 2.332(2) - Cd(1)-O(2): 2.332(2) - Cd(1)-O(3): 2.3311(2) - Cd(1)-O(3)#1: 2.3311(2) - Cd(1)-N(4): 2.317(2) - Cd(1)-N(4)#1: 2.317(2) - O(2)-Cd(1)-O(2)#1: 91.76(7) - O(3)-Cd(1)-O(2)#1: 88.24(7) - O(3)-Cd(1)-O(2): 88.24(7) - Cd(2)-O(1): 2.1892(2) - Cd(2)-O(3): 2.5890(2) - Cd(2)-O(4): 2.3173(2) - Cd(2)-N(1): 2.403(2) - Cd(2)-N(3): 2.261(2) - Cd(2)-N(6)#2: 2.315(2) - N(3)-Cd(2)-N(1): 71.37(7) - N(3)-Cd(2)-N(6)#2: 162.10(8) - N(6)#2-Cd(2)-O(3): 111.72(7)

Compound 2: - Mn(1)-O(1): 2.1653(2) - Mn(1)-O(4)#1: 2.1804(2) - Mn(1)-O(5): 2.2175(2) - Mn(1)-N(2): 2.223(2) - Mn(1)-N(3): 2.260(2) - O(4)#1-Mn(1)-O(5): 95.96(7) - O(1)-Mn(1)-O(5): 92.42(7) - O(1)-Mn(1)-O(4)#1: 87.72(7) - N(3)-Mn(1)-O(5): 164.70(7) - N(3)-Mn(1)-O(4)#1: 97.24(7) - N(2)-Mn(1)-O(1): 135.52(7) - N(2)-Mn(1)-N(3): 75.62(7) - N(3)-Mn(1)-O(1): 95.80(7) - N(2)-Mn(1)-O(5): 89.48(7) - N(2)-Mn(1)-O(4)#1: 136.25(7)

Symmetry transformations used to generate equivalent atoms:
For 1: #1: 1-x, 1-y, 1-z; #2: -1/2+x, 1/2-y, -1/2+z
For 2: #1: x, y, -1+z

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

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