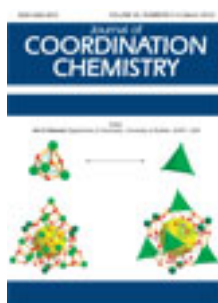


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Zinc(II) complexes of 4,4-oxybis(benzoate) and 2-propyl-4,5-imidazoledicarboxylic acid with bipyridine

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Zinc(II) complexes of 4,4-oxybis(benzoate) and 2-propyl-4,5-imidazoledicarboxylic acid with bipyridine

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The reactions of dicarboxylic acids, such as 4,4-oxybis(benzoic acid) [H₂oba] and 2-propyl-4,5-imidazoledicarboxylate [H₃pimdc], under hydrothermal conditions in the presence of an appropriate zinc salt yield two mononuclear complexes, which are characterized by elemental analysis, infrared spectrum, electrochemical analysis, thermal analysis, and X-ray crystal diffraction. Complex **1**, [Zn(Hoba)₂(4,4'-bpy)₂], forms a 2-D supramolecular layer like rhombus *via* hydrogen bonds (O–H···N). Complex **2**, [Zn(H₂pimdc)₂(2,2'-bpy)]·H₂O, forms a zig-zag chain *via* multiple hydrogen bonds and C–H···π interactions. The moderate hydrogen-bond interactions in **1** and **2** play an important role for structural stability. The electrochemical analyses of **1** and **2** reveal electron transfer of **1** is reversible and **2** is quasi-reversible.

Keywords: Electrochemical analysis; Thermal analysis; X-ray crystal diffraction; Hydrogen bonds; C–H···π interactions

1. Introduction

Design of diverse topologies in supramolecular chemistry and crystal engineering has attracted attention [1]. An effective strategy is to select building blocks with diverse donors as directing nodes to assemble multi-dimensional frameworks by binding metal centers [2]. Self-assembly is the molecular recognition process adopted by nature to generate the elegant and intricate molecular machinery from which life is built. Various weak dispersive interactions, such as hydrogen bonds, π–π stacking, hydrophobic, charge transfer, electrostatic, and metal ion coordination, represent the backbone of self-assembly processes [3]. Conventional strong hydrogen bonds are of fundamental importance in molecular recognition and crystal engineering involving organic systems. Besides these conventional strong hydrogen bonds, varieties of unconventional intermolecular interactions are also instrumental in determining the supramolecular structure of organic solids [4–6]. Investigations on benzenecarboxylates have been

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enhanced by the use of benzenecarboxylate-derivatives and heterocyclic carboxylic acids such as 4,4-oxybis(benzoic acid) and imidazolecarboxylic acids [7]. Structural characterizations of polymeric H₂oba complexes with diverse topologies have been reported, such as threefold pcu-type network, double-helical chain [8], 3-D microporous metal-organic frameworks [9], single-stranded helical chain [10], guest-free porous framework [11], pillared-layer related structure [12], and other architectures [13–16]. A convenient path to polymeric structures uses a bifunctional ligand, 4,4'-bpy, to link metal ions in an infinite configuration [17]. Some supramolecular H₂oba and 4,4'-bpy complexes with diverse topologies have been synthesized, their coordinated cations are Ag(I) [18], Cu(II) [19, 20], and Co(II) [21]. Polymeric H₃pimdc complexes are not many. Recently, Li and co-workers [22] reported a 2-D coordination polymer with 2-propyl-4,5-imidazoledicarboxylate and 1,3-bis(4-pyridyl)propane(bpp), [Cd₂(Hpimdc)₂(bpp)(H₂O)]_n.

In this article, we have combined the advantages of the hydrothermal method of synthesis and multi-functional carboxylic acids in the presence of 2,2'-bpy/4,4'-bpy to form two new coordination complexes, [Zn(C₁₄H₉O₅)₂(C₁₀H₈N₂)₂] (**1**) and [Zn(C₈H₉N₂O₄)₂(C₁₀H₈N₂)]·H₂O (**2**), by employing 4,4-oxybis(benzoic acid) and 2-propyl-4,5-imidazoledicarboxylate. Observing from the *c*-axis, **1** forms a distorted square plane with [Hoba][−] and 4,4'-bpy *via* hydrogen bonds (O–H···N); **2** forms a zig-zag chain *via* multiple hydrogen bonds and C–H···π interactions.

2. Experimental

All chemicals were obtained from commercial sources and used as received. Solvents were purified. Infrared (IR) spectra were recorded in KBr pellets using a Nicolet 520 FT-IR spectrophotometer. Elemental analyses (C, H, and N) were performed on a Perkin-Elmer 2400 II elemental analyzer. A Perkin-Elmer Diamond TG/DTA thermal analyzer was used to record TG curves in static air at a heating rate of 10°C min^{−1}/20°C min^{−1} from 25°C to 900°C using platinum crucibles.

2.1. Preparation of [Zn(Hoba)₂(4,4'-bpy)₂] (**1**)

H₂oba (0.2582 g, 1 mmol) was dissolved in 20 mL *N,N*-dimethylformamide (DMF) at room temperature and the pH was adjusted to 6.5 with triethylamine. Zn(CH₃COO)₂·2H₂O (0.2195 g, 1 mmol) was dissolved in 10 mL methanol and 25 mL distilled water, the two solutions were mixed, 4,4'-bpy (0.1562 g, 1 mmol) was added, stirred, and heated to 75°C for 8 h. Then the filtered solution was evaporated at room temperature for 20 days, giving highly pure and well-shaped colorless block crystals which were washed with distilled water (yield: 71.3%). Elemental Anal. Calcd for C₄₈H₃₄ZnN₄O₁₀ (%): C, 64.62; H, 3.84; N, 6.28. Found (%): C, 64.70; H, 3.86; N, 6.23. IR (KBr, cm^{−1}): 3425(s), 3075(s), 3047(s), 2973(m), 1927(vs), 1687(s), 1637(s), 1600(vs), 1538(s), 1504(s), 1414(s), 1352(s), 1309(s), 1244(vs), 1213(s), 1158(s), 1099(s), 1071(s), 1049(s), 1158(s), 1009(s), 879(s), 860(s), 805(s), 780(s), 694(m), 669(m), 641(m).

2.2. Preparation of $[Zn(H_2pimdc)_2(2,2'-bpy)] \cdot H_2O$ (**2**)

H_3pimdc (0.1986 g, 1 mmol) was dissolved in 40 mL distilled water at room temperature and the pH was adjusted to 8 with triethylamine. $ZnCl_2$ (0.0687 g, 0.5 mmol) was dissolved in 15 mL methanol, the two solutions were mixed, 2,2'-bpy (0.0781 g, 0.5 mmol) was added, stirred, and heated to 75°C for 8 h. Then the filtered solution was evaporated at room temperature for 10 days to give highly pure and well-shaped colorless block crystals which were washed with distilled water (yield: 76.3%). Elemental Anal. Calcd for $C_{26}H_{28}ZnN_6O_9$ (%): C, 49.26; H, 4.45; N, 13.26. Found (%): C, 49.23; H, 4.48; N, 13.23. IR (KBr, cm^{-1}): 3524(m), 3489(w), 3035(m), 2967(m), 2930(m), 2874(m), 1727(s), 1708(m), 1618(m), 1594(m), 1557(m), 1532(vs), 1479(vs), 1439(s), 1393(s), 1340(m), 1315(m), 1281(s), 1228(m), 1152(m), 1102(w), 1050(m), 1024(s), 972(m), 898(m), 830(m), 764(s), 740(m), 654(m), 595(w), 514(s).

2.3. X-ray data collection and structure refinement

A high quality crystal of the complex was selected and mounted on a glass fiber. The data were collected on a Bruker SMART CCD diffractometer at 296(2) K. Graphite-monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) and the ω scan technique were used to collect the data sets. Absorption corrections were applied using SADABS [23]. The crystal structure was solved with direct methods and refined with a full-matrix least-squares technique using the SHELXTL package [24]. Anisotropic thermal parameters were applied to all non-hydrogen atoms. Hydrogen atoms were generated geometrically. The crystallographic data as well as details of the data collection and refinement for the complex are listed in table 1. Selected bond lengths and angles are given in table 2.

3. Results and discussion

3.1. Crystal structure descriptions

Complex **1** crystallizes in the *monoclinic* space group of $C2/c$. In the asymmetric unit of **1**, there are one Zn(II), two $[Hoba]^-$, and two bridging 4,4'-bpy. Each Zn(II) is four-coordinate by two N1 from two 4,4'-bpy and two O1 of carboxylates from two $[Hoba]^-$ (figure 1). Selected molecular geometry parameters are listed in table 2 and hydrogen-bond parameters are listed in table 3. The coordination geometry around Zn(II), comprising N_2O_2 from two $[Hoba]^-$ anions and two bpy ligands, can be described as a high distorted square planar. Two Zn(II) ions are linked by a $[Hoba]^-$ and a bpy; the Zn–N distance is 2.063(2) Å and the Zn–O distance is 1.919(2) Å. The $[Hoba]^-$ and bpy are connected *via* O4–H \cdots N2 hydrogen bond; the O4–H \cdots N2 distance is 1.85 Å (see table 3). From the 100 plane, **1** forms a 2-D network structure *via* hydrogen bonds forming a supramolecular layer (see figure 2).

Complex **2** crystallizes in the *orthorhombic* space group $Pbca$. In **2**, each Zn(II) is six-coordinate by two oxygen atoms and two nitrogen atoms of two $[H_2pimdc]^-$ and two nitrogen atoms of a 2,2'-bpy. The geometry around zinc(II) can be described as a distorted octahedron; the Zn–N distances are in the 2.151(3)–2.167(2) Å range (table 2)

Table 1. Crystal data and structure refinements for **1** and **2**.

	1	2
Complexes		
Empirical formula	C ₄₈ H ₃₄ ZnN ₄ O ₁₀	C ₂₆ H ₂₈ ZnN ₆ O ₉
Formula weight	892.16	633.91
Temperature (K)	296(2)	296(2)
Crystal system	Monoclinic	Orthorhombic
Space group	C2/c	Pbca
Unit cell dimensions (Å, °)		
<i>a</i>	31.46(2)	10.481(4)
<i>b</i>	7.293(5)	18.070(7)
<i>c</i>	26.896(15)	29.570(11)
α	90	90
β	138.24(4)	90
γ	90	90
Volume (Å ³), <i>Z</i>	4110(4), 4	5600(4), 8
Calculated density (g cm ⁻³)	1.442	1.504
Absorption coefficient (mm ⁻¹)	0.665	0.941
<i>F</i> (000)	1840	2624
Crystal size (mm ³)	0.41 × 0.39 × 0.37	0.41 × 0.39 × 0.36
θ range for data collection (°)	1.53–25.01	2.25–25.01
Data/restraints/parameters	3623/0/285	4932/2/381
Goodness-of-fit on <i>F</i> ²	1.076	1.002
Final <i>R</i> ^a indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0327, <i>wR</i> ₂ = 0.0934	<i>R</i> ₁ = 0.0378, <i>wR</i> ₂ = 0.1087
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0371, <i>wR</i> ₂ = 0.0956	<i>R</i> ₁ = 0.0531, <i>wR</i> ₂ = 0.1208
Largest difference peak and hole (e Å ⁻³)	0.239 and -0.244	0.551 and -0.306

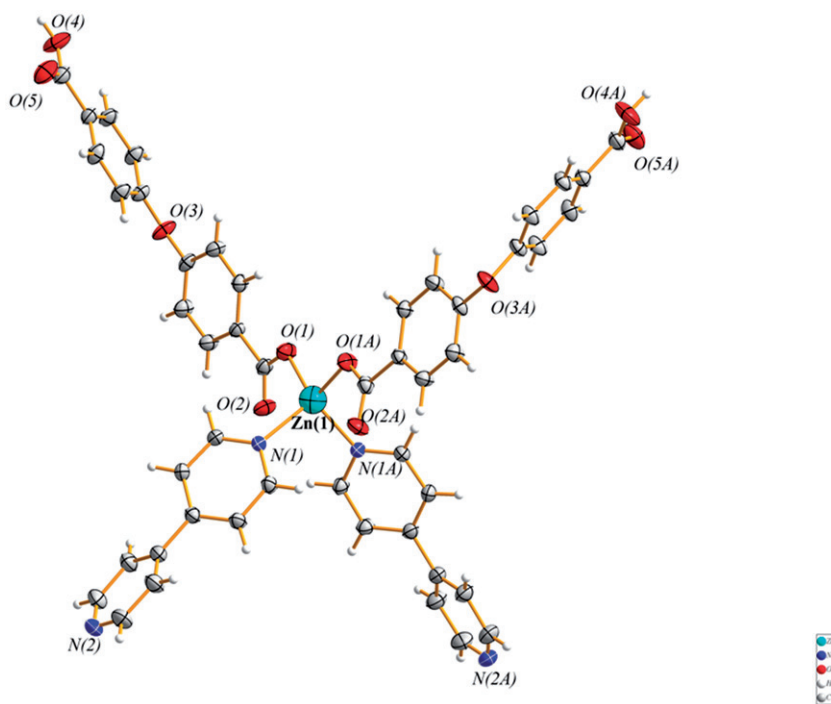
$$^a R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|, wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)]^{1/2}.$$

Table 2. Selected bond lengths (Å) and angles (°) for **1** and **2**.

1			
Zn(1)–O(1)	1.919(2)	O(1)–Zn(1)–N(1)	107.63(8)
Zn(1)–N(1)	2.063(2)	O(1)#1–Zn(1)–N(1)	122.24(8)
O(1)–Zn(1)–O(1)#1	100.23(11)	N(1)–Zn(1)–N(1)#1	98.59(10)
2			
Zn(1)–N(5)	2.123(3)	O(1)–Zn(1)–N(6)	90.16(10)
Zn(1)–O(1)	2.142(2)	N(2)–Zn(1)–N(6)	101.68(9)
Zn(1)–N(2)	2.143(2)	N(5)–Zn(1)–O(5)	95.91(10)
Zn(1)–N(6)	2.151(3)	O(1)–Zn(1)–O(5)	97.39(9)
Zn(1)–O(5)	2.166(2)	N(2)–Zn(1)–O(5)	77.74(8)
Zn(1)–N(4)	2.167(2)	N(6)–Zn(1)–O(5)	172.37(10)
N(5)–Zn(1)–O(1)	166.55(10)	N(5)–Zn(1)–N(4)	101.18(9)
N(5)–Zn(1)–N(2)	97.65(10)	O(1)–Zn(1)–N(4)	77.36(8)
O(1)–Zn(1)–N(2)	87.13(9)	N(2)–Zn(1)–N(4)	157.40(9)
N(5)–Zn(1)–N(6)	76.58(11)	N(6)–Zn(1)–N(4)	94.79(9)
O(5)–Zn(1)–N(4)	87.94(8)		

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

and the Zn–O distances are 2.142(2) Å and 2.166(2) Å. The Zn–N and Zn–O distances of **2** are longer than those for **1**. The molecular structure of **2** is depicted in figure 3. The structure contains hydrogen bonds and C–H... π interactions with four kinds of hydrogen bonds. The first is water molecules of crystallization *via* hydrogen-bonding between the N3 and O9, the second is between O3...H/O7...H and O2/O6 from the

Figure 1. View of coordination environment of **1** with thermal ellipsoid at 30% probability.Table 3. Hydrogen-bonding geometries for **1** and **2**.

D–H...A	Symmetry code	D–H (Å)	H...A (Å)	D...A (Å)	D–H...A (°)
Compound 1					
O(4)–H(4A)···N(2)	$-x + 1/2, y + 5/2, -z + 1/2$	0.82	1.85	2.663(3)	170.7
Compound 2					
O(9)–H(9B)···O(8)	$x - 1/2, -y + 3/2, -z + 2$	0.82	2.04	2.824(3)	159.3
O(9)–H(9A)···O(5)	$-x + 3/2, y + 1/2, z$	0.82	2.20	2.989(4)	164.2
N(3)–H(3A)···O(9)	$-x + 1, y - 1/2, -z + 3/2$	0.86	1.91	2.761(3)	170.1
N(1)–H(1)···O(2)	$-x + 1, -y + 1, -z + 2$	0.86	2.06	2.903(3)	167.6
O(7)–H(7)···O(6)		0.82	1.67	2.492(4)	179.3
O(14)–H(14E)···O(13)		0.82	1.73	2.554(3)	179.5

carbonyl group in the same $H_3\text{pimdc}$, the third is between N1–H from a imidazole of $[\text{Zn}(\text{H}_2\text{pimdc})_2(2,2'\text{-bpy})] \cdot \text{H}_2\text{O}$ and O2 from the carbonyl of a neighboring $[\text{Zn}(\text{H}_2\text{pimdc})_2(2,2'\text{-bpy})] \cdot \text{H}_2\text{O}$, the last is O9–H9A···O5 and O9–H9B···O8 (figure 4a) with distance shown in table 3. The C–H··· π interactions play an important role in supramolecular structure of **2** with distances of C–H··· π interactions 2.923, 2.528, 3.005, 2.578, 2.781, 2.804 (figure 4b) and 2.879 Å (figure 4c). The propyl groups have no disorder because of C–H··· π interactions. Complex **2** forms a 1-D chain (figure 4d) *via* C–H··· π interactions and hydrogen bonds. From the *c*-axis **2** forms a

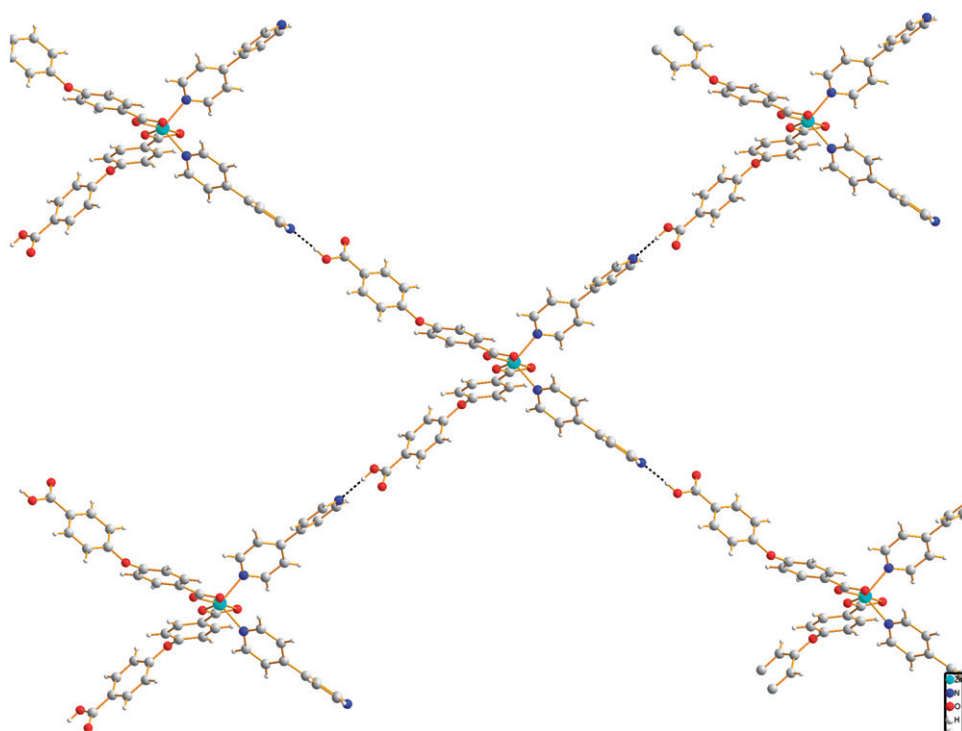


Figure 2. The 2-D layer *via* hydrogen bonds along the 100 axis and 100 plane in 1.

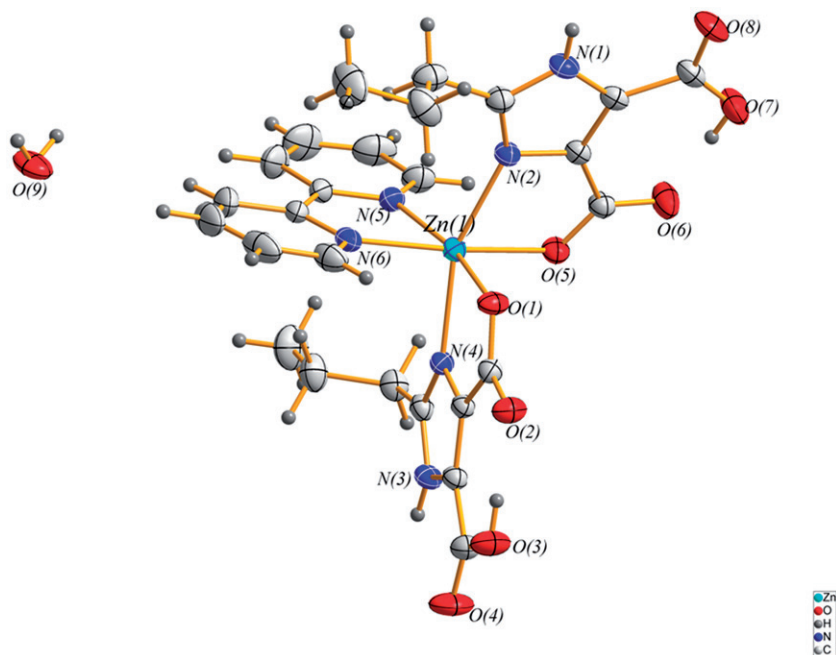


Figure 3. View of coordination environment of 2 with thermal ellipsoid at 30% probability.

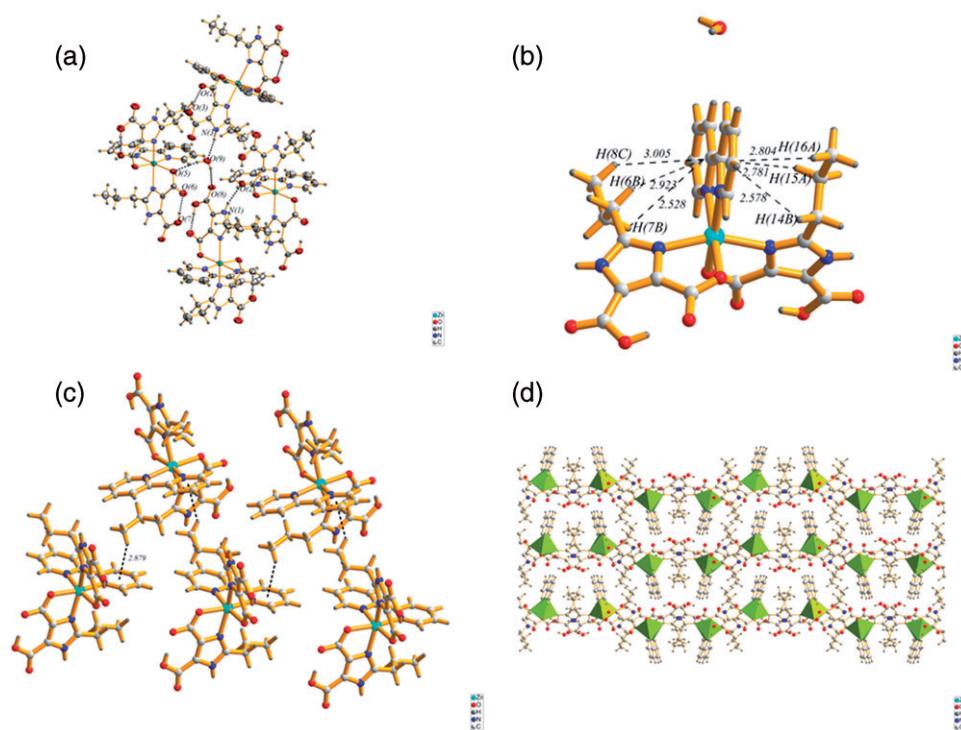


Figure 4. View of (a) the crystal packing of **2** showing the O–H...O hydrogen bonds (displacement ellipsoids are drawn at the 30% probability level and the hydrogen bonds are indicated by dashed lines); (b) and (c) the C–H... π stacking interactions of **2**; (d) the 1-D chain topology of **2** with balls or sticks.

zig-zag topology *via* intermolecular hydrogen bonds and C–H... π stacking interactions forming a 3-D solid-state structure (figure 4c).

3.2. Spectroscopic properties

Complexes **1** and **2** are air stable. IR spectra show features attributable to each component of **1** [25] with characteristic bands of carboxylates in the usual region at 1687–1637 cm^{-1} for the antisymmetric stretch and at 1414–1352 cm^{-1} for the symmetric stretch. IR spectra show features attributable to each component of **2** and characteristic bands of carboxylates are in the usual region at 1727–1708 cm^{-1} for the antisymmetric stretch and at 1479–1393 cm^{-1} for the symmetric stretch. The $\Delta\nu$ values [$\Delta\nu = \nu_{\text{as}}(\text{COO}^-) - \nu_{\text{s}}(\text{COO}^-)$] are 273 and 285 cm^{-1} for **1** and 246 and 415 cm^{-1} for **2**, suggesting unidentate carboxylates [26], consistent with the crystal structures. Very strong absorptions at 1588 cm^{-1} and 1552 cm^{-1} are assigned to C=N of 4,4'-bpy and 2,2'-bpy, respectively. In the complexes, these C=N bands shift higher by 50 cm^{-1} for **1** and 20 cm^{-1} for **2**. The shift suggests that the nitrogen coordinates to the metal [27]. The IR results indicate that the ligands coordinate to metal *via* oxygen of the carboxyl and nitrogen of bpy.

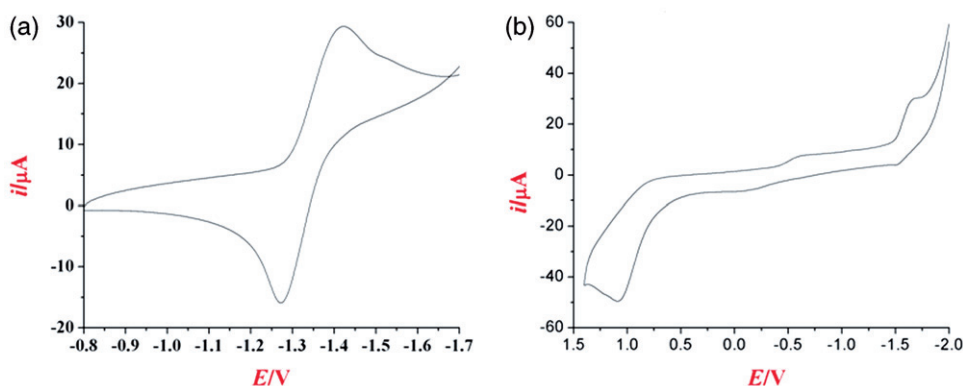


Figure 5. Cyclic voltammograms of **1** and **2**; scan rate: 100 mV s^{-1} .

3.3. Electrochemical analysis

Complexes **1** and **2** were dissolved in distilled water and DMF at room temperature at $3.8 \times 10^{-4} \text{ mol L}^{-1}$ and $9.6 \times 10^{-4} \text{ mol L}^{-1}$, respectively, for electrochemical studies with modified glassy carbon electrodes (GC, $\varphi = 2.0 \text{ mm}$) in 0.05 mol L^{-1} lithium perchlorate ($\text{pH} = 11.66$) aqueous solution at room temperature under nitrogen at a scan rate of 100 mV s^{-1} . As shown in figure 5(a), **1** showed a reversible redox couple in water and DMF medium, which could be attributed to redox of Zn(II)/Zn(0) [28], and the mean peak potential $E_{1/2} = (E_{\text{pa}} + E_{\text{pc}})/2$ was -1.344 V . From $\Delta E(0.142 \text{ V})$ and $I_{\text{pa}}/I_{\text{pc}} (-0.54)$, the electron transfer is reversible. Complex **1** is an electroactive substance in this solution. For **2**, a quasi-reversible redox peak attributed to redox of Zn(II)/Zn(0) was observed, as shown in figure 5(b). The mean peak potential $E_{1/2} = (E_{\text{pa}} + E_{\text{pc}})/2$ was 240 mV for **2**.

Caution: The pH value was measured by pH-meter.

3.4. Thermal analysis

TG curves of **1** with a heating rate of $10^\circ\text{C min}^{-1}$ are shown in figure 6(a). Complex **1** undergoes decomposition in three stages. The first stage at $225.7\text{--}273.7^\circ\text{C}$ corresponds to release of one $[\text{Hoba}]^-$ from $[\text{Zn}(\text{Hoba})_2(4,4'\text{-bpy})_2]$ with weight loss of 28.8% (Calcd 28.83%). The second stage occurs at $273.7\text{--}384.0^\circ\text{C}$ with mass loss of 34.0% (Calcd 35.0%) that correlate with elimination of two $4,4'\text{-bpy}$. The third stage occurs at $439.4\text{--}504.1^\circ\text{C}$ corresponding to loss of a $4\text{-phenoxybenzaldehyde}$ with mass loss of 20.8% (actual value: 22.2%).

The TG curves of **2** with a heating rate of $20^\circ\text{C min}^{-1}$ are shown in figure 6(b). Complex **2** undergoes decomposition in three stages, the first from 117°C to 208°C with mass loss of 2.8% (Calcd 2.84%) for elimination of water. The second stage takes place at $208\text{--}336.4^\circ\text{C}$ from release of one $[\text{H}_2\text{pimdc}]^-$ and one $2,2'\text{-bpy}$ with weight loss of 55.9% (Calcd 55.74%). The third stage occurs at $336.4\text{--}552.6^\circ\text{C}$ corresponding to loss of a $2\text{-propyl-1 } H\text{-imidazole}$ for **2** with mass loss of 15.4% (actual value: 17.37%).

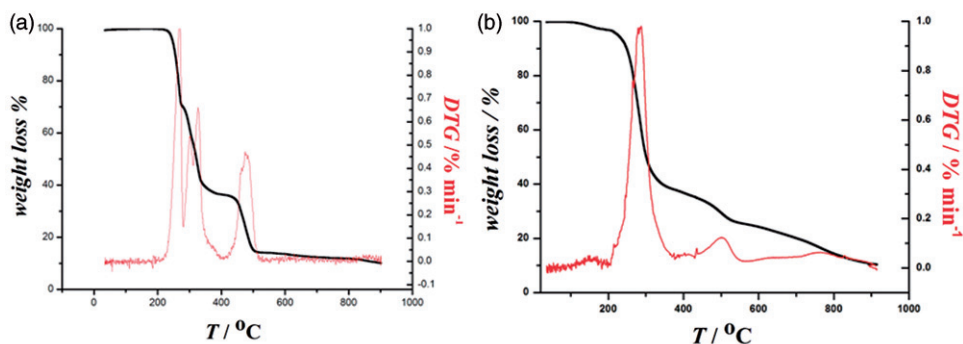


Figure 6. The TG-DTG curves of **1** and **2**.

4. Conclusion

The synthesis and characterization of two new Zn(II) complexes, $[\text{Zn}(\text{Hoba})_2(4,4'\text{-bpy})_2]$ and $[\text{Zn}(\text{H}_2\text{pimdc})_2(2,2'\text{-bpy})] \cdot \text{H}_2\text{O}$, by spectral method (IR), elemental analysis, thermal analysis (TG), electrochemical analysis, and single-crystal X-ray diffraction techniques are reported. Complex **1** forms a 2-D network *via* hydrogen bonds ($\text{O4-H} \cdots \text{N2}$) and coordination of 4,4'-bpy and H_2oba . Complex **2** forms a zig-zag geometry *via* multiple hydrogen bonds, $\text{C-H} \cdots \pi$ interactions, and coordination of 2,2'-bpy and H_3pimdc . In **2**, strong hydrogen bonds among an uncoordinated water molecule, carboxylates, and N-H of the imidazoles and $\text{C-H} \cdots \pi$ interactions play important roles in the 3-D network. IR spectra of **1** and **2** indicate unidentate carboxylate. Electrochemical analyses of **1** and **2** show **1** to be electroactive in this solution. Analyses of synthetic conditions, structures, and coordination modes of Zn(II) reveal that solvent, pH, and structures of ligands have important effects on the coordination modes of Zn(II).

Supplementary material

CCDC 782184 and 787626 contain the supplementary crystallographic data for this article. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

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