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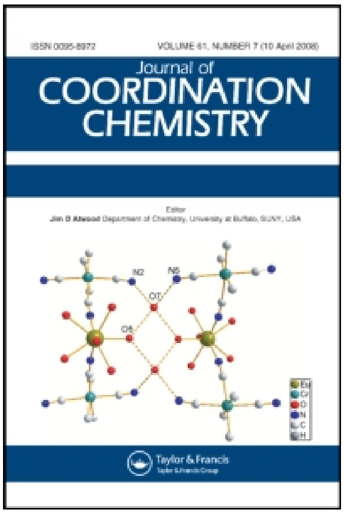

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Self-assembly of three 1-D zinc-benzenedicarboxylate coordination polymers with 1,10-phenanthroline

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Self-assembly of three 1-D zinc–benzenedicarboxylate coordination polymers with 1,10-phenanthroline

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Three zinc(II) benzenedicarboxylate coordination polymers, $\{Zn^{II}(L_1)(phen)(H_2O)\}_n$ (**1**), $\{[Zn^{II}(L_2)(phen)]_2\}_n$ (**2**), and $\{[Zn^{II}(L_3)(phen)(H_2O)]\}_n$ (**3**) ($L_1 = $ 1,4-benzenedicarboxylic dianion, $L_2 = $ 1,3-benzenedicarboxylic dianion, $L_3 = $ 1,2-benzenedicarboxylic dianion, and phen = 1,10-phenanthroline), have been synthesized by self-assembly. Structural analyses of **1**–**3** reveal that the compounds are one-dimensional (1-D) chains. However, the structural motifs for **1**–**3** are distinct from each other, where **1** forms 1-D zig-zag chains, **2** is in 1-D ladder-like motif, and **3** is a 1-D helical form. Compounds **1**–**3** exhibit photoluminescence with emission maxima at *ca* 371, 392, and 375 nm, respectively.

Keywords: 1-D coordination polymer; Zinc complex; Benzenedicarboxylic acid; 1,10-Phenanthroline

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1. Introduction

Self-assembly of coordination polymers with coordination bonds, hydrogen bonds, $\pi \cdots \pi$ packing interactions, have attracted great scientific attention [1–8]. Development of coordination polymers is important for intriguing topological structures and unexpected properties for applications in materials chemistry, such as gas sorption, storage, and separations [9, 10], heterogeneous catalysis [11, 12], molecular recognition [13], luminescence [14], nonlinear optics [15], and magnetic properties [16].

Selection of multidentate ligand to link metal ions is important for building coordination polymers. Benzenedicarboxylic acids (such as 1,2-benzenedicarboxylic acid, 1,3-benzenedicarboxylic acid, and 1,4-benzenedicarboxylic acid) and their dianions have been used, because they can lead to varieties of multi-dimensional coordination polymers and benzenedicarboxylic acids have rigid aromatic spacers making them special for interesting electronic and magnetic interactions between the metal ions through conjugative interaction [17–21]. Terminal ligands play an important role in the topology and property of the coordination polymers.

Herein, we report syntheses, crystal structures, and photoluminescent properties of three Zn^{II}-benzenedicarboxylate coordination polymers, $\{Zn^{II}(L_1)(phen)(H_2O)\}_n$ (**1**),

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$\{[Zn^{II}(L_2)(phen)]_2\}_n$ (**2**), and $\{[Zn^{II}(L_3)(phen)(H_2O)]\}_n$ (**3**) (L_1 = 1,4-benzenedicarboxylic dianion, L_2 = 1,3-benzenedicarboxylic dianion, and L_3 = 1,2-benzenedicarboxylic dianion, and phen = 1,10-phenanthroline), all of which are 1-D infinite chains; **1** is a 1-D zigzag chain, while **2** is a 1-D ladder, and **3** a 1-D helical structure.

2. Experimental

2.1. *Materials and general methods*

All reagents were obtained commercially analytical grade and used without purification; all manipulations were carried out at ambient conditions. Elemental C, H, and N analyses were performed on a Perkin Elmer analyzer. Infrared spectra were recorded as KBr pellets on a Bruker EQUIN0X 55 IR spectrometer.

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2.2. *Syntheses of 1–3*

2.2.1. $\{Zn^{II}(L_1)(phen)(H_2O)\}_n$ (1). A mixture of $ZnCl_2$ (0.136 g, 1 mmol) in water (10 mL), terephthalic acid (1,4-benzenedicarboxylic acid, 0.166 g, 1 mmol), and 1,10-phenanthroline (0.198 g, 1 mmol) in DMF (10 mL) was added into a Teflon-steel autoclave inside a programmable electric furnace reactor. Mixed-solvo-thermal reaction lasted for about 12 h at 423.15 K, and then cooled to room temperature naturally. Colorless crystals of **1** were obtained (yield: about 74% based on Zn). Anal. Calcd for **1** (%), C, 56.11; H, 3.16; and N, 6.55; Found (%), C, 56.14; H, 3.22; and N, 6.50. IR (KBr): 3419 s, 1592 s, 1517 s, 1426 s, 1386 s, 1308 m, 1223 w, 1145 w, 1104 m, 1090 s, 1049 w, 1017 w, 867 m, 841 s, 814 m, 725 s, 644 m, and 557 m.

2.2.2. $\{[Zn^{II}(L_2)(phen)]_2\}_n$ (2). A mixture of $ZnCl_2$ (0.136 g, 1 mmol) in water (10 mL), isophthalic acid (1,3-benzenedicarboxylic acid, 0.166 g, 1 mmol), and 1,10-phenanthroline (0.198 g, 1 mmol) in methanol (10 mL) was added into a Teflon-steel autoclave inside a programmable electric furnace reactor. Mixed-solvothermal reaction lasted for 12 h at 423.15 K, and then it was cooled to room temperature naturally. Colorless crystals of **2** were obtained (yield: about 68% based on Zn). Anal. Calcd for **2** (%), C, 58.58; H, 2.95; and N, 6.83; Found (%), C, 58.74; H, 3.01; and N, 6.79. IR (KBr): 1614.78 s, 1560.49 s, 1514.14 m, 1492.39 m, 1436.84 m, 1424.47 s, 1377.84 s, 1271.63 w, 1159.45 w, 1101.03 w, 1075.53 w, 849.26 m, 745.04 m, and 718.77 s.

2.2.3. $\{[Zn^{II}(L_3)(phen)(H_2O)]\}_n$ (3). A mixture of $ZnCl_2$ (0.136 g, 1 mmol) in water (10 mL), potassium hydrogen phthalate (0.204 g, 1 mmol), and 1,10-phenanthroline (0.198 g, 1 mmol) in methanol (10 mL) was added into a Teflon-steel autoclave inside a programmable electric furnace reactor. Mixed-solvo-thermal reaction lasted for 12 h at 423.15 K, and then cooled to room temperature naturally. Colorless crystals of **3** were obtained (yield: about 63% based on Zn). Anal. Calcd for **3** (%), C, 53.85; H, 3.60; and N, 6.29; Found (%), C, 53.97; H, 3.68; and N, 6.40. IR (KBr): 3388.42 s, 1679.62 m,

Table 1. Crystallographic data and structure refinement summary for **1**–**3**.

	1	**2**	**3**
Empirical formula	$C_{20}H_{14}N_2O_5Zn$	$C_{20}H_{12}N_2\ O_4Zn$	$C_{20}H_{16}N_2O_6Zn$
Mr	427.70	409.69	445.74
Temperature (K)	290(2)	290(2)	290(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P–1*	*P2/c*	$P2_1/n$
Unit cell dimensions (Å, °)			
a	9.1860(1)	8.6473(4)	9.6294(1)
b	10.5830(1)	10.2374(5)	8.9676(1)
c	11.5683(2)	18.3921(9)	21.3832(3)
α	114.704(1)		
β	91.538(1)	99.605(1)	90.735(1)
γ	115.114(1)		
Volume (Å^3), Z	896.14(2), 2	1605.35(13), 4	1846.34(4), 4
Calculated density (g cm^{-3})	1.585	1.695	1.604
Crystal size (mm^3)	0.28 × 0.25 × 0.22	0.28 × 0.24 × 0.20	0.26 × 0.24 × 0.18
θ range for data collection (°)	2.00–28.30	1.99–28.30	1.90–28.30
Reflections collected	13147	15932	20781
Independent reflection	4419 [R(int) = 0.0178]	3976 [R(int) = 0.0300]	4591 [R(int) = 0.0370]
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.063	1.035	1.007
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0240$, $wR_2 = 0.0651$	$R_1 = 0.0275$, $wR_2 = 0.0650$	$R_1 = 0.0409$, $wR_2 = 0.0923$
R indices (all data)	$R_1 = 0.0274$, $wR_2 = 0.0663$	$R_1 = 0.0378$, $wR_2 = 0.0694$	$R_1 = 0.0847$, $wR_2 = 0.1070$
Largest difference peak and hole (e Å^{-3})	0.339 and −0.225	0.313 and −0.285	0.861 and −0.333

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1595.73 s, 176.21 s, 11557.83 s, 1517.88 s, 1485.97 m, 1448.68 w, 1382.83 s, 1255.97 m, 1103.81 w, 866.78 m, 851.96 m, 791.95 m, and 728.07 s.

2.3. *Crystallographic data collection and structure determination*

Single crystal X-ray diffraction studies of **1**–**3** were performed on a Bruker SMART diffractometer equipped with a charge coupled device (CCD) area detector with a graphite monochromator situated in the incident beam for data collection. The determination of unit cell parameters and data collections were performed with Mo-Kα radiation ($\lambda = 0.71073$ Å) by ω scan mode in the range of $2.00 \leq \theta \leq 28.30$ (for **1**), $1.99 \leq \theta \leq 28.30$ (for **2**), and $1.90 \leq \theta \leq 28.30$ (for **3**) at 293(2) K. All data were corrected by semi-empirical methods using SADABS. SAINT [22] was used for integration of the diffraction profiles.

All structures were solved by direct methods using SHELXS of the SHELXTL-97 package and refined with SHELXL [23]. Zinc was located from E-maps and other non-hydrogen atoms were located in successive difference Fourier syntheses. The final refinements were performed by full matrix least-squares methods with anisotropic thermal parameters for non-hydrogen atoms on F^2. Hydrogens of the ligands were generated theoretically onto the specific atoms and refined isotropically with fixed thermal factors. Hydrogens of coordinated water were partially located using the

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

Zn(1)–O(1)	2.0517(11)	O(2)–C(13)	1.2702(18)	N(1)–C(1)	1.3308(19)
Zn(1)–O(2)	2.0265(10)	O(3)–C(13)	1.2437(18)	N(1)–C(12)	1.3572(19)
Zn(1)–O(4)	2.0028(10)	O(4)–C(17)	1.2606(17)	N(2)–C(10)	1.325(2)
Zn(1)–N(1)	2.1099(12)	O(5)–C(17)	1.2394(17)	N(2)–C(11)	1.3533(19)
Zn(1)–N(2)	2.1797(12)	C(16)–C(15)#1	1.386(2)	C(19)–C(20)#2	1.388(2)
O(2)–Zn(1)–O(1)	87.49(5)	O(4)–Zn(1)–N(1)	101.39(5)	C(13)–O(2)–Zn(1)	124.63(10)
O(4)–Zn(1)–O(1)	130.94(4)	O(1)–Zn(1)–N(2)	90.99(5)	C(17)–O(4)–Zn(1)	112.25(9)
O(4)–Zn(1)–O(2)	97.37(5)	O(2)–Zn(1)–N(2)	165.03(5)	C(1)–N(1)–Zn(1)	126.55(11)
N(1)–Zn(1)–N(2)	77.75(5)	O(4)–Zn(1)–N(2)	94.87(5)	C(12)–N(1)–Zn(1)	114.61(9)
O(1)–Zn(1)–N(1)	127.38(5)	C(11)–N(2)–Zn(1)	112.38(10)	C(10)–N(2)–Zn(1)	128.90(11)
O(2)–Zn(1)–N(1)	91.36(5)				

Symmetry transformations used to generate equivalent atoms: #1: $-x+3$, $-y+1$, $-z+2$; #2: $-x+1$, $-y$, $-z+1$.

Table 3. Selected bond lengths (Å) and angles (°) for **2**.

Zn(1)–O(1)	2.035(1)	O(1)–C(13)	1.242(2)	N(1)–C(1)	1.326(3)
Zn(1)–O(2)#2	2.026(1)	O(2)–C(13)	1.263(2)	N(1)–C(12)	1.351(2)
Zn(1)–O(3)#1	2.005(1)	O(3)–C(20)	1.270(3)	N(2)–C(10)	1.324(2)
Zn(1)–N(1)	2.194(2)	O(4)–C(20)	1.234(3)	N(2)–C(11)	1.361(2)
Zn(1)–N(2)	2.155(2)				
O(2)#2–Zn(1)–O(1)	96.29(6)	O(1)–Zn(1)–N(2)	126.79(6)	C(1)–N(1)–Zn(1)	127.2(1)
O(3)#1–Zn(1)–O(1)	97.42(6)	O(2)#2–Zn(1)–N(2)	93.08(5)	C(12)–N(1)–Zn(1)	114.1(1)
O(3)#1–Zn(1)–O(2)#2	101.74(6)	O(3)#1–Zn(1)–N(2)	131.46(6)	C(10)–N(2)–Zn(1)	126.6(1)
O(1)–Zn(1)–N(1)	83.16(6)	C(13)–O(1)–Zn(1)	163.2(1)	C(11)–N(2)–Zn(1)	114.8(1)
O(2)#2–Zn(1)–N(1)	165.68(6)	C(13)–O(2)–Zn(1)#2	120.0(1)	C(1)–N(1)–C(12)	118.6(2)
O(3)#1–Zn(1)–N(1)	92.50(6)	C(20)–O(3)–Zn(1)#1	105.9(1)	C(10)–N(2)–C(11)	118.2(2)
N(2)–Zn(1)–N(1)	76.14(6)				

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

Table 4. Selected bond lengths (Å) and angles (°) for **3**.

Zn(1)–N(1)	2.155(2)	Zn(1)–O(5)	2.115(1)	C(13)–O(1)	1.273(2)
Zn(1)–N(2)	2.136(2)	N(1)–C(1)	1.331(3)	C(13)–O(2)	1.229(2)
Zn(1)–O(1)	1.996(1)	N(1)–C(12)	1.351(2)	C(20)–O(3)	1.245(2)
Zn(1)–O(3)#1	2.394(1)	N(2)–C(10)	1.320(3)	C(20)–O(4)	1.270(2)
Zn(1)–O(4)#1	2.121(1)	N(2)–C(11)	1.359(2)		
O(1)–Zn(1)–O(3)#1	160.5(5)	O(1)–Zn(1)–N(1)	104.56(6)	N(2)–Zn(1)–N(1)	77.30(6)
O(1)–Zn(1)–O(4)#1	105.23(5)	O(1)–Zn(1)–N(2)	102.67(6)	O(3)–C(20)–O(4)	121.9(1)
O(1)–Zn(1)–O(5)	88.68(6)	O(5)–Zn(1)–N(2)	90.41(6)	O(4)–C(20)–C(19)	119.0(2)
O(4)#1–Zn(1)–O(3)#1	57.88(5)	N(1)–Zn(1)–O(3)#1	86.61(5)	O(3)–C(20)–C(19)	119.1(2)
O(5)–Zn(1)–O(3)#1	83.62(6)	N(2)–Zn(1)–O(3)#1	95.28(5)	C(13)–O(1)–Zn(1)	119.2(1)
O(5)–Zn(1)–O(4)#1	94.79(5)	O(4)#1–Zn(1)–N(2)	151.71(6)	C(20)–O(4)–Zn(1)#2	96.0(1)
O(5)–Zn(1)–N(1)	163.53(6)	O(4)#1–Zn(1)–N(1)	91.17(6)	C(20)–O(3)–Zn(1)#2	84.2(1)

Symmetry transformations used to generate equivalent atoms: #1: $-x+3/2$, $y+1/2$, $-z+1/2$; #2: $-x+3/2$, $y-1/2$, $-z+1/2$.

difference Fourier method or generated theoretically. Further crystallographic data and experimental details for structural analyses of the complexes are summarized in table 1, and selected bond lengths and angles with their estimated standard deviations for **1**–**3** in tables 2–4, respectively.

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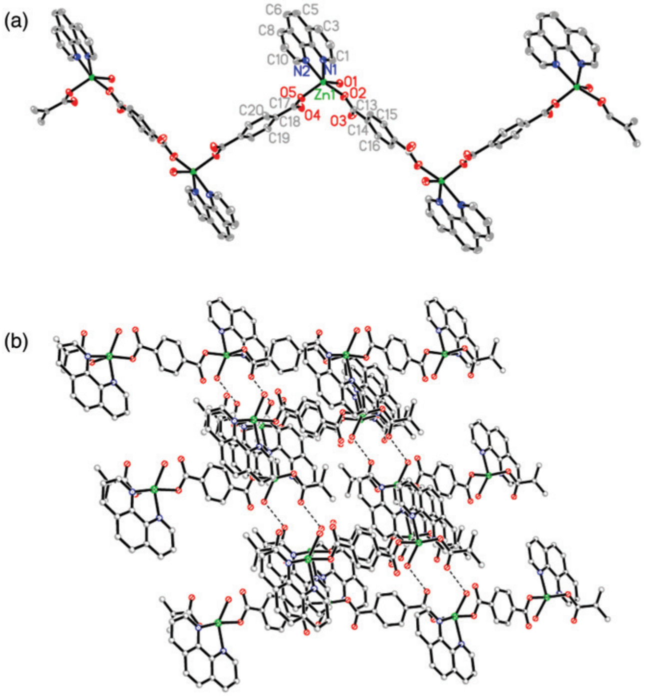

Figure 1. (a) Perspective view of the asymmetry unit and the zigzag chain of **1**; (b) crystal packing diagram of **1** along the *b* axis showing the hydrogen-bond and $\pi\cdots\pi$ packing interactions between 1-D chains.

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3. Results and discussion

3.1. *Description of the crystal structures of 1–3*

3.1.1. $\{Zn^{II}(L_1)(phen)(H_2O)\}_n$ (1). Single crystal X-ray determination reveals that **1** is composed of 1-D neutral zigzag chains. In each asymmetric unit of **1**, one Zn^{II} is coordinated by (1) 1,10-phenanthroline with Zn–N distances of 2.11(1)–2.178(1) Å, (2) two oxygens from two carboxylates of two 1,4-benzenedicarboxylates with Zn–O distances of 2.003(1)–2.027(1) Å, and (3) one water with Zn–O distance of 2.052(1) Å, forming a pyramid-like coordination sphere, as shown in figure 1(a). Two neighboring Zn^{II} centers are connected by a 1,4-benzenedicarboxylate, forming a straightforward block. Unlike the coordination polymer previously reported, which also contains zinc and 1,4-benzenedicarboxylate [24] in **1**, 1,10-phenanthroline instead of 4,4–biprydine is used, forming the 1-D zigzag chain as shown in figure 1(b).

Analysis of the crystal packing of **1** indicates that there are two independent $O–H\cdots O$ hydrogen bonds, and two types of $\pi\cdots\pi$ packing interactions. The $O–H\cdots O$ hydrogen bonds include intra-chain hydrogen bonds and inter-chain hydrogen bonds, with the former formed by coordinated water with the uncoordinated oxygen of 1,4-benzenedicarboxylate in the same chain with the $D\cdots A$ distance 2.612(2) Å and O–H–O angle 147.6°. Inter-chain $O–H\cdots O$ hydrogen bond is formed by coordinated water with the uncoordinated oxygen from 1,4-benzenedicarboxylate of

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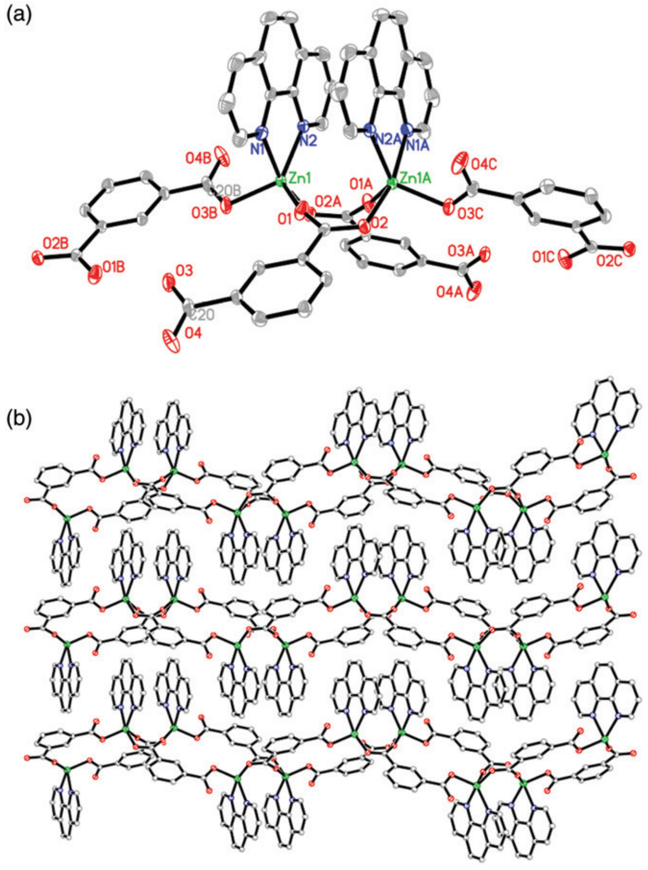

Figure 2. (a) Perspective view of the binuclear unit of **2**; (b) the 1-D ladder-like chain and crystal packing diagram of **2** along the *a* axis showing two kinds of $\pi \cdots \pi$ packing interactions in the crystal of **2**.

an adjacent chain with D$\cdots$A distance 2.699(2) Å and O–H–O angle of 176.7°. The distance between two planes of adjacent 1,10-phenanthrolines in two neighboring chains is 3.552 Å and the distance between 1,10-phenanthroline and 1,4-benzenedicarboxylate of the neighboring chain is 3.341 Å; both distances are within the range of $\pi \cdots \pi$ packing interactions 3.3–3.7 Å. The inter-chains O–H$\cdots$O hydrogen bonds and $\pi \cdots \pi$ packing interactions link these 1-D chains into 3-D crystal of **1**, as depicted in figure 1(b).

3.1.2. $\{[Zn^{II}(L_2)(phen)]_2\}_n$ (2).

Single crystal X-ray determination reveals that **2** is composed of 1-D neutral ladder-like chains. In each unit of **2**, there are two equivalent Zn^{II}'s and each Zn^{II} is coordinated by 1,10-phenanthroline with Zn–N distances of 2.155(2)–2.194(2) Å, and three oxygens from three carboxylates of three 1,3-benzenedicarboxylates with Zn–O distances of 2.005(1)–2.035(1) Å, forming a pyramid-like coordination sphere, as shown in figure 2(a). Two neighboring Zn^{II} centers are chelated by two carboxylates of two 1,3-benzenedicarboxylates to form a dinuclear node with

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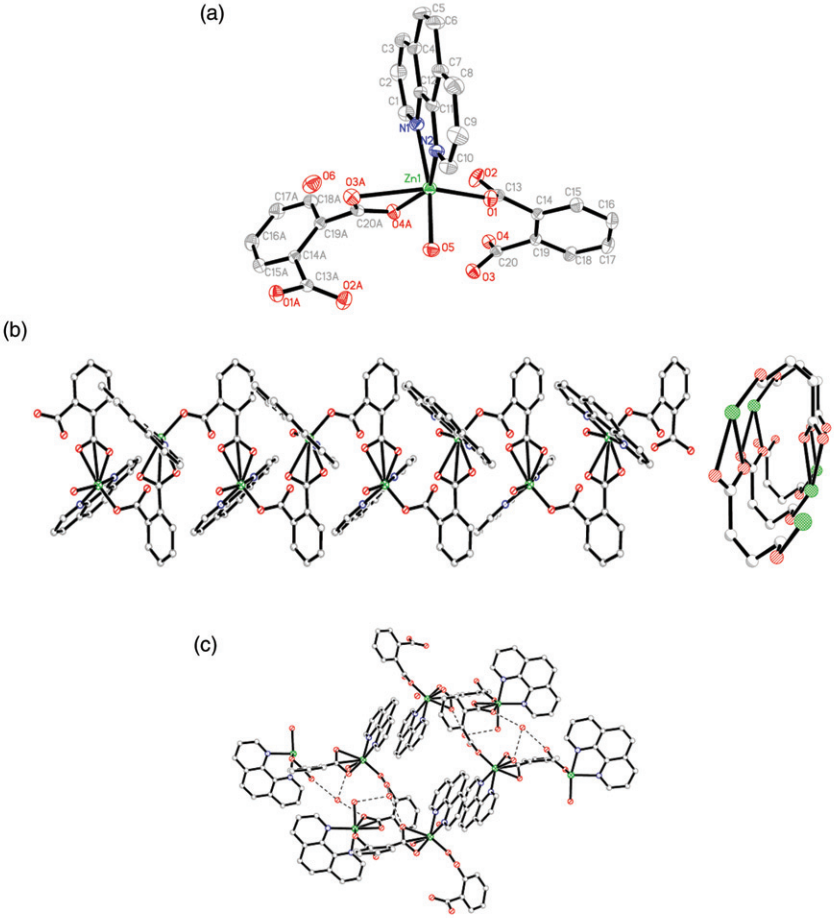

Figure 3. (a) Perspective view of the asymmetric unit of **3**; (b) perspective view of the 1-D helical chain in **3**; and (c) crystal packing diagram of **3** showing the $\pi \cdots \pi$ packing interactions between two neighboring chains in the crystal of **3**.

Zn$\cdots$Zn distance of 3.896(2) Å. The dinuclear nodes are connected by four 1,3-benzenedicarboxylates, which act as a long bridge through benzene, along the *c* axis to from a 1-D ladder-like infinite chain (figure 2b).

Analysis of the crystal packing of **2** indicates that there are two kinds of $\pi \cdots \pi$ packing interactions, intra-chain $\pi \cdots \pi$ packing, and inter-chain $\pi \cdots \pi$ packing interactions. The distance between two planes of two adjacent 1,10-phenanthrolines in a dinuclear node, i.e., intra-chain $\pi \cdots \pi$ packing distance, is 3.477 Å and the distance between two adjacent 1,10-phenanthrolines of two neighboring chains, i.e., inter-chain $\pi \cdots \pi$ packing distance, is about 3.392 Å, both within the range of $\pi \cdots \pi$ packing interactions. The inter-chain $\pi \cdots \pi$ packing interactions link these 1-D chains into the 3-D crystal of **2**, as depicted in figure 2(b).

3.1.3. $\{[Zn^{II}(L_3)(phen)(H_2O)]\}_n$ (3).

Single crystal X-ray determination reveals that **3** is composed of 1-D neutral helical chains. In **3**, each Zn(II) is coordinated by (1)

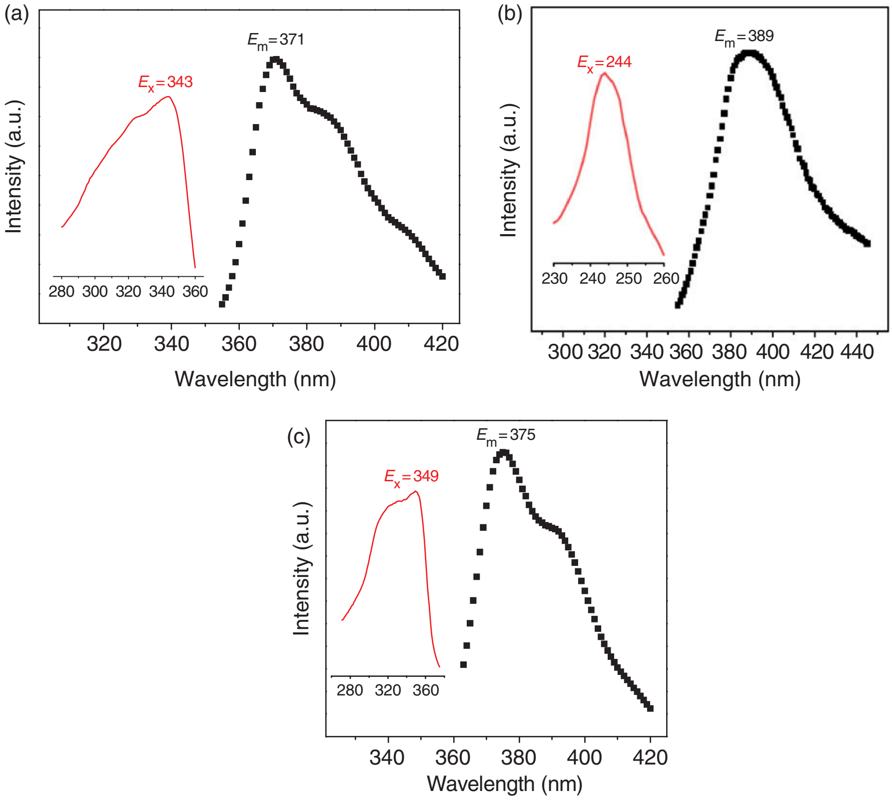

Figure 4. Fluorescence emission spectra in the solid state at room temperature for: (a) **1**, (b) **2**, and (c) **3**.

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1,10-phenanthroline with Zn–N distances of 2.136(2)–2.155(2) Å, (2) three oxygens from two carboxylates of two 1,2-benzenedicarboxylates with Zn–O distances of 1.996(1)–2.394(1) Å, and (3) one coordinated water with Zn–O distance of 2.115(1) Å forming an octahedral coordination sphere as shown in figure 3(a). Neighboring Zn(II) units are connected by a 1,2-benzenedicarboxylate at 5.977(6) Å to form a 1-D infinite chain (figure 3b). The 1,10-phenanthrolines as terminal ligands prevent the chain spread, and inner-chain hydrogen bonds formed by coordinated water with oxygen from the 1,2-benzenedicarboxylates make the chain into a helical form (figure 3b).

Analysis of the crystal packing of **3** indicates that there is a kind of $\pi \cdots \pi$ packing interaction between two 1-D helical chains formed by two adjacent 1,10-phenanthrolines from two neighboring chains with average distance of about 3.350 Å, which is within the range of $\pi \cdots \pi$ packing interactions. The inter-chains $\pi \cdots \pi$ packing interactions link these 1-D chains into the 3-D crystal of **3**, as depicted in figure 3(c).

3.2. *Fluorescence properties*

Solid state fluorescence properties of **1**–**3** have been measured at room temperature. Emission spectra displayed in figure 4 exhibit that all three complexes possess fluorescence properties. As shown in figure 4(a), a fluorescence emission peak at 371 nm was observed for **1** ($\lambda_{ex} = 343$ nm). Excited at 244 nm, **2** displays a fluorescence emission at 389 nm (figure 4b) and **3** displays a fluorescence emission peak at 375 nm when excited at 249 nm (figure 4c). Benzenedicarboxylic acids and 1,10-phenanthroline display fluorescence emission peaks at about 362 and 380 nm, respectively. Since Zn(II) is d^{10} fluorescence of **1**–**3** may be attributed to metal-to-ligand charge transfer (MLCT).

4. Conclusion

Three zinc-benzenedicarboxylate coordination polymers have been prepared by self-assembly and structurally characterized by X-ray diffraction. The structures show 1-D infinite chains in 1-D zigzag, 1-D ladder-like, and 1-D helical forms, respectively. Photoluminescence studies of the three complexes show that they exhibit fluorescent emission bands at *ca* 371, 389, and 375 nm, respectively.

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Supplementary material

Crystallographic data for the crystal structures reported in this article have been deposited with the Cambridge Crystallographic Data Center, CCDC nos 641649, 657099, and 657100. These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223-336033; or Email: deposit@ccdc.cam.ac.uk).

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References

[1] B.F. Hoskins, R. Robson. *J. Am. Chem. Soc.*, **111**, 5962 (1989).
[2] B.F. Abrahams, B.F. Hoskins, D.M. Michail, R. Robson. *Nature*, **369**, 727 (1994).
[3] O.M. Yaghi, G. Li, H. Li. *Nature*, **378**, 703 (1995).
[4] S. Kitagawa, R. Kitaura, S.-I. Noro. *Angew. Chem. Int. Ed.*, **43**, 2334 (2004).
[5] J.L.C. Rowsell, E.C. Spencer, J. Eckert, J.A.K. Howard, O.M. Yaghi. *Science*, **309**, 1350 (2005).
[6] G. Férey, C. Mellot-Draznieks, C. Serre, F. Millange, J. Dutour, S. Surble, I. Margiolaki. *Science*, **309**, 2040 (2005).
[7] S. Bureekaew, S. Horike, M. Higuchi, M. Mizuno, T. Kawamura, D. Tanaka, N. Yanai, S. Kitagawa. *Nat. Mater.*, **8**, 831 (2009).
[8] Q. Li, W. Zhang, O.S. Miljanić, C.-H. Sue, Y.-L. Zhao, L. Liu, C.B. Knobler, J.F. Stoddart, O.M. Yaghi. *Science*, **3025**, 855 (2009).

[9] N.L. Rosi, J. Eckert, M. Eddaoudi, D.T. Vodak, J. Kim, M. O'Keeffe, O.M. Yaghi. *Science*, **300**, 1127 (2003).

[10] R. Banerjee, A. Phen, B. Wang, C. Knobler, H. Furukawa, O.M. Yaghi. *Science*, **319**, 939 (2008).

[11] J.S. Seo, D. Whang, H. Lee, S.I. Jun, J. Oh, Y.J. Jeon, K. Kim. *Nature*, **404**, 982 (2000).

[12] C.-D. Wu, A. Hu, L. Zhang, W. Lin. *J. Am. Chem. Soc.*, **127**, 8940 (2005).

[13] R.-G. Xiong, X.-Z. You, B.F. Abrahams, Z. Xue, C.-M. Che. *Angew. Chem. Int. Ed.*, **40**, 4422 (2001).

[14] S.Y. Yu, Z.X. Zhang, E.C.-C. Cheng, Y.Z. Li, V.W.-W. Yam, H.P. Huang, R. Zhang. *J. Am. Chem. Soc.*, **127**, 1799 (2005).

[15] Z. Guo, R. Cao, X. Wang, H. Li, W. Yuan, G. Wang, H. Wu, J. Li. *J. Am. Chem. Soc.*, **131**, 6894 (2009).

[16] W. Kaneko, S. Kitagawa, M. Ohba. *J. Am. Chem. Soc.*, **129**, 248 (2007).

[17] W. Chen, J.Y. Wang, C. Chen, Q. Yue, H.M. Yuan, J.S. Chen, S.N. Wang. *Inorg. Chem.*, **42**, 944 (2003).

[18] B. Zhai, W.Z. Shen, X.Y. Chen, H.B. Song, W. Shi, P. Cheng. *Inorg. Chem. Commun.*, **9**, 1293 (2006).

[19] P.-Z. Li, X.-M. Lu, X.-Z. Yang. *Inorg. Chim. Acta*, **361**, 293 (2008).

[20] X.-M. Lu, P.-Z. Li, X.-T. Wang, S. Gao, X.-J. Wang, S. Wang, Y.-H. Deng, Y.-J. Zhang, L. Zhou. *Polyhedron*, **27**, 2402 (2008).

[21] X.-M. Lu, P.-Z. Li, X.-T. Wang, S. Gao, X.-J. Wang, L. Zhou, C.-S. Liu, X.-N. Sui, J.-H. Feng, Y.-H. Deng, Q.-H. Jin, J. Liu, N. Liu, J.-P. Lian. *Polyhedron*, **27**, 3669 (2008).

[22] Bruker AXS. *SAINT Software Reference Manual*, Madison, WI, USA (1998).

[23] G.M. Sheldrick. *SHELXTL NT (Version 5.1) Program for Solution and Refinement of Crystal Structures*, University of Göttingen, Göttingen, Germany (1997).

[24] D. Feng, S.-X. Liu, P. Sun, F.-J. Ma, W. Zhang. *J. Coord. Chem.*, **63**, 1737 (2010).

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