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# Synthesis, Crystal Structure, and Properties of Two Zinc Tubular Coordination Polymers Based on Fluconazole

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*Two Zn(II)-containing complexes based on fluconazole,  $\{[Zn(HFlu)_2(IPA)] \cdot 9H_2O\}_n$  (1),  $\{[Zn(HFlu)_2(OH-BDC)] \cdot 8H_2O\}_n$  (2) (HFlu = fluconazole; 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol;  $H_2IPA$  = isophthalic acid;  $OH-H_2BDC$  = 5-hydroxyisophthalic acid) have been synthesized and structurally characterized. Complex 1 and 2 are both a one-dimensional (1D) tubular structure with the distorted dinuclear zinc rectangular-shaped cavity, and large free water molecules involved in strong  $O-H \cdots O$  and  $O-H \cdots N$  hydrogen bonds are accommodated in the 1D tubular structure. The thermal stabilities and photoluminescent properties of the coordination polymers have also been investigated.*

**Keywords** Fluconazole; fluorescence; one-dimension tube; thermal properties

## Introduction

Design and synthesis of metal–organic coordination polymers have rapidly developed in recent years, owing to their fascinating structures with potential applications in catalysis, luminescence, ion exchange, and gas storage [1–8]. Therefore, a search of rational synthetic strategies for metal–organic complexes is an important task. One of the possible ways involves the use of ligands with numerous coordination sites. Fluconazole [2-(2,4-difluorophenyl)-1,3-di(1H-1,2,4-triazol-1-yl)propan-2-ol] known as an antifungal drug was first synthesized and reported in the scientific literature by Richardson et al. [9,10]. However, Fluconazole shows interesting coordinating characteristics to afford extended networks in a head-to-tail mode with good flexibility through rotating and twisting the C–C and C–N bonds when coordinating to metal ions [11–14]. Besides, fluconazole could chelate to metal ions with endodentate nitrogen atoms ( $N^2$ ) and alkoxo atom to form binuclear complex [15]. Another reason of the HFlu ligand proved to be a good candidate to construct polymeric structure is that it has several available donors/acceptors (2,4-difluorophenyl and hydroxyl groups) to form various weak interactions to stabilize the supramolecular frameworks [11–21].

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In this context, we report two novel coordination polymers,  $\{[\text{Zn}(\text{HFlu})_2(\text{IPA})]\cdot 9\text{H}_2\text{O}\}_n$  (**1**),  $\{[\text{Zn}(\text{HFlu})_2(\text{OH-BDC})]\cdot 8\text{H}_2\text{O}\}_n$  (**2**). (HFlu = fluconazole, 2-(2,4-difluoro-phenyl)-1,3-bis(1,2,4-triazol-1-yl)-propan-2-ol); OH-H<sub>2</sub>BDC = 5-hydroxyisophthalic acid; H<sub>2</sub>IPA = isophthalic acid). Single-crystal X-ray analysis reveals that Complex **1** and **2** are both a one-dimensional (1D) tubular structure with the distorted dinuclear zinc rectangular-shaped cavity and large free water molecules involved in strong O—H...O and O—H...N hydrogen bonds are accommodated in the 1D tubular structure. The fluorescence and thermal gravimetric of these complexes have also been studied.

## Experimental

### Materials and Instrumentation

All chemicals were commercial materials of analytical grade and used as received. The Fourier transform infrared spectroscopy (FTIR) spectrum was obtained on a Nicolet 520 FT-IR spectrophotometer (Waltham, Massachusetts) by Fourier transform methods in the 4000–400 cm<sup>−1</sup> regions, using KBr pellets. Emission spectra were taken using a Perkin-Elmer LS55 fluorescence spectrometer (Waltham, Massachusetts). Elemental analysis for C, H, N was carried out on a Perkin-Elmer 2400 II elemental analyzer. Thermogravimetric analysis (TGA) was performed on a Perkin-Elmer TG/DTA 6300 thermal analyzer (Waltham, Massachusetts) under N<sub>2</sub> atmosphere at a heating rate of 10°C min<sup>−1</sup> in the temperature range 30°C–1000°C.

### Preparation of $\{[\text{Zn}(\text{HFlu})_2(\text{IPA})]\cdot 9\text{H}_2\text{O}\}_n$ (**1**)

A mixture of fluconazole (153 mg, 0.5 mmol), isophthalic acid (83 mg, 0.5 mmol), ZnCl<sub>2</sub> (136 mg, 1.0 mmol), 17 mL H<sub>2</sub>O, and 2 mL ethanol was sealed in a 30 mL Teflon-lined stainless-steel container. An aqueous solution of sodium hydroxide was added dropwise with stirring to adjust the pH value of the solution to 6.0. The mixture was kept under autogenous pressure at 150°C for 3 days before cooling to room temperature at a rate of 5°C hr<sup>−1</sup>. Transparent crystals of **1** were obtained, washed with alcohol three times, and dried in a vacuum desiccator using silicagel (yield: 62.8% based on Zn). Elemental analysis (%) for C<sub>34</sub>H<sub>46</sub>F<sub>4</sub>N<sub>12</sub>O<sub>15</sub>Zn: calcd. C 40.67, H 4.62, N 16.74; found: C 40.56, H 4.65, N 16.69. IR (KBr, cm<sup>−1</sup>): 3480 s, 3117 m, 1616 s, 1540 s, 1419 m, 1374 m, 1320 m, 1385 s, 1277 s, 1260 w, 1129 s, 1111 w, 993 w, 862 m, 655 m.

### Preparation of $\{[\text{Zn}(\text{HFlu})_2(\text{OH-BDC})]\cdot 8\text{H}_2\text{O}\}_n$ (**2**)

The same synthetic procedure as that for **1** was used except that isophthalic acid (83 mg, 0.5 mmol) was replaced by 5-hydroxyisophthalic acid (91 mg, 0.5 mmol) (yield: 73.1% based on Zn). Elemental analysis (%) for C<sub>34</sub>H<sub>44</sub>F<sub>4</sub>N<sub>12</sub>O<sub>15</sub>Zn: calcd. C 40.75, H 4.43, N 16.77; found: C 40.64, H 4.49, N 16.66. IR (KBr, cm<sup>−1</sup>): 3446 s, 3392 s, 3143 m, 1617 m, 1575 s, 1506 w, 1419 m, 1376 m, 1275 m, 1134 m, 1118 w, 984 w, 780 m, 735 w, 676 m, 654 w.

### X-Ray Data Collection and Structure Refinement

X-ray diffraction data for the complex were collected on a Bruker SMART CCD diffractometer equipped with graphite-monochromatized MoK $\alpha$  radiation ( $\lambda = 0.71073$  Å) at

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

Compounds	<b>1</b>	<b>2</b>
Empirical formula	C <sub>34</sub> H <sub>46</sub> F <sub>4</sub> N <sub>12</sub> O <sub>15</sub> Zn	C <sub>34</sub> H <sub>44</sub> F <sub>4</sub> N <sub>12</sub> O <sub>15</sub> Zn
Formula weight	1004.20	1002.19
Temperature (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	<i>P</i> <sub>1</sub>	<i>P</i> <sub>1</sub>
<i>a</i> (Å)	10.0496(4)	10.0834(3)
<i>b</i> (Å)	11.66550(10)	11.5734(6)
<i>c</i> (Å)	20.1805(5)	19.9550(5)
$\alpha$ (°)	82.5480(10)	82.325(3)
$\beta$ (°)	76.2480(10)	76.352(3)
$\gamma$ (°)	75.036(2)	75.774(3)
Volume, <i>Z</i> (Å <sup>3</sup> )	2214.19(11), 2	2186.51(14), 2
Calculated density (g cm <sup>-3</sup> )	1.50	1.519
Absorption coefficient (mm <sup>-1</sup> )	0.651	0.659
<i>F</i> (000)	1032	1032
Crystal size (mm <sup>3</sup> )	0.32 × 0.22 × 0.20	0.33 × 0.24 × 0.22
$\theta$ range for data collection (°)	1.81–25.00	1.82–25.00
Data/restraints/parameters	7705/37/616	7590/19/608
Goodness of fit on <i>F</i> <sup>2</sup>	1.041	1.030
<i>R</i> <sub>1</sub> / <i>wR</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0355/0.1011	0.0382/0.1019
<i>R</i> <sub>1</sub> / <i>wR</i> <sub>2</sub> (all data)	0.0422/0.1050	0.0470/0.1080
Largest difference peak/hole (e Å <sup>-3</sup> )	0.619/−0.421	0.733/−0.350

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

296(2) K. A high-quality crystal of the complex was selected and was mounted on a glass fiber. Collect the datasets with the  $\omega$  scan technique. Empirical absorption corrections were applied using the SADABS program [22]. The structure was solved by direct methods and all non-hydrogen atoms were refined with anisotropic thermal parameters by a full-matrix least square based on *F*<sup>2</sup> using SHELXTL package [23]. All non-hydrogen atoms were refined anisotropically. Further refinement details of the structural analysis for the two complexes are given in Table 1. Selected bond lengths and angles of the complexes are listed in Table 2, and possible selected hydrogen bond geometries are given in Table 3.

## Results and Discussion

### Crystal Structure Descriptions

Single-crystal X-ray study of **1** exhibits a 1D coordination polymer constructed by the connection of Zn<sup>2+</sup>. The complex **1** crystallizes in the triclinic space group *P*<sub>1</sub>, and the asymmetric unit contains one Zn(II) ion, two HFlu ligands, one IPA<sup>2-</sup> ligand, and nine free water molecules in a crystal lattice. The coordination environment of Zn(II) ion in **1** is shown in Fig. 1(a). Each Zn(II) ion is six-coordinated by three oxygen atoms of two carboxylates

**Table 2.** Selected bond lengths (Å) and angles (°) for complex **1** and **2<sup>a</sup>**

<b>1</b>			
Zn(1)-O(1)	2.0212(16)	N(5)#1-Zn(1)-N(11)	178.00(7)
Zn(1)-N(1)	2.1247(19)	O(1)-Zn(1)-O(3)#2	91.21(7)
Zn(1)-N(5)#1	2.1370(18)	N(1)-Zn(1)-O(3)#2	147.02(7)
Zn(1)-N(11)	2.1762(18)	N(5)#1-Zn(1)-O(3)#2	91.25(7)
Zn(1)-O(3)#2	2.2046(18)	N(11)-Zn(1)-O(3)#2	88.54(7)
Zn(1)-O(4)#2	2.2996(16)	O(1)-Zn(1)-O(4)#2	149.07(7)
O(1)-Zn(1)-N(1)	121.19(7)	N(1)-Zn(1)-O(4)#2	89.29(7)
O(1)-Zn(1)-N(5)#1	93.34(7)	N(5)#1-Zn(1)-O(4)#2	90.06(7)
N(1)-Zn(1)-N(5)#1	92.69(7)	N(11)-Zn(1)-O(4)#2	88.14(6)
O(1)-Zn(1)-N(11)	88.66(7)	O(3)#2-Zn(1)-O(4)#2	57.97(6)
N(1)-Zn(1)-N(11)	86.41(7)		
<b>2<sup>a</sup></b>			
Zn(1)-O(2)#1	2.051(2)	N(7)-Zn(1)-N(1)	85.75(8)
Zn(1)-N(12)#2	2.120(2)	O(2)#1-Zn(1)-O(5)	89.69(8)
Zn(1)-N(7)	2.144(2)	N(12)#2-Zn(1)-O(5)	91.34(8)
Zn(1)-N(1)	2.148(2)	N(7)-Zn(1)-O(5)	145.05(7)
Zn(1)-O(5)	2.2078(18)	N(1)-Zn(1)-O(5)	89.68(7)
Zn(1)-O(4)	2.3613(18)	O(2)#1-Zn(1)-O(4)	146.71(8)
O(2)#1-Zn(1)-N(12)#2	93.46(8)	N(12)#2-Zn(1)-O(4)	89.39(7)
O(2)#1-Zn(1)-N(7)	124.85(9)	N(7)-Zn(1)-O(4)	88.16(7)
N(12)#2-Zn(1)-N(7)	91.59(8)	N(1)-Zn(1)-O(4)	88.49(7)
O(2)#1-Zn(1)-N(1)	89.73(8)	O(5)-Zn(1)-O(4)	57.06(6)
N(12)#2-Zn(1)-N(1)	176.65(8)		

<sup>a</sup>Symmetry transformations used to generate equivalent atoms for **1**: #1  $-x + 2, -y + 1, -z + 1$ ; #2  $x + 1, y, z$ ; for **2**: #1  $x + 1, y, z$ ; #2  $-x, -y + 1, -z + 1$ .

from two different IPA<sup>2+</sup> ligands and three nitrogen atoms from three HFlu molecules, leading to a distorted octahedron geometry. The Zn–N and Zn–O bond lengths are in the range of 2.1247(19)–2.1762(18) and 2.0212(16)–2.2996(16), respectively. While virtually identical to the values reported for {[Zn(HFlu)<sub>2</sub>(Suc)(H<sub>2</sub>O)<sub>2</sub>]}·H<sub>2</sub>O, these bond lengths are slightly different from the reported compound [Zn(HFlu)(TPA)]<sub>n</sub> [24]. This is attributed to the increase in the coordination number of the metallic centers (in [Zn(HFlu)(TPA)]<sub>n</sub> the Zn<sup>2+</sup> metal centers were five-coordinated). The two neighboring Zn(II) centers are connected by four bridging triazolyl group of two different fluconazole ligands, which results in the formation of a distorted dinuclear zinc rectangular-shaped cavity of size 7.883 × 5.637 Å<sup>2</sup>, labeled as [Zn(1)-C(11)-Zn(1B)-C(11B)] (Fig. 1(b)). It is worthy of note that there are four fluconazole ligands linked to the dinuclear zinc rectangular-shaped cavity, but two exo-triazolyl groups of the other fluconazoles were not coordinated to the Zn(II) ion. The Zn–Zn distances connected two adjacent Zn atoms by fluconazole ligands are 10.355 Å. The two adjacent dinuclear zinc rectangular-shaped cavities are further connected by bridging carboxylate group ions of H<sub>2</sub>IPA ligands, generating a 1D tube (Fig. 2). Each carboxylate group of the H<sub>2</sub>dpa ligands is completely deprotonated, and the two completely deprotonated carboxylate groups adopt bidentate chelating and monodentate coordination modes, respectively. The Zn–Zn distance connected two adjacent Zn atoms by IPA<sup>2+</sup> ligands

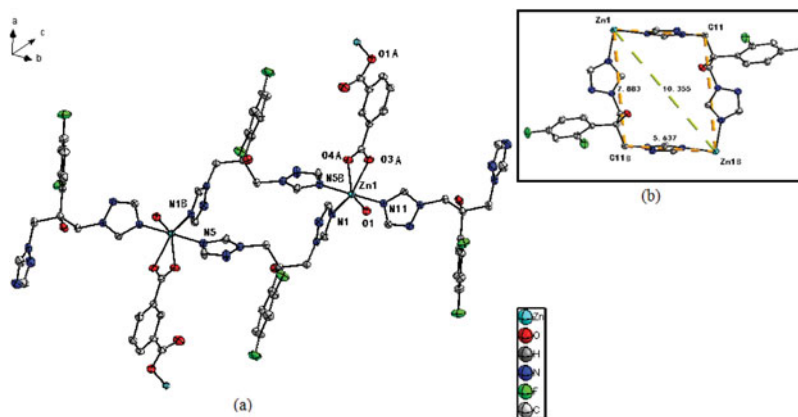
**Table 3.** Selected hydrogen-bonding geometries for **1** and **2**<sup>a</sup>

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<(DHA) (°)
Complex <b>1</b>				
O6-H6...O10#1	0.82	1.90	2.711(3)	173.2
O8-H8D...N12#2	0.85	2.20	2.915(3)	141.5
O8-H8C...O9	0.85	1.90	2.742(3)	174.3
O9-H9C...O2#1	0.85	1.89	2.731(3)	173.2
O9-H9D...O13#1	0.85	1.93	2.773(3)	173.2
O10-H10C...O11#1	0.85	1.97	2.816(3)	170.6
O10-H10D...O13#1	0.85	2.15	2.990(3)	170.9
O11-H11E...O8	0.85	1.84	2.689(3)	177.7
O11-H11F...N3#3	0.85	2.17	3.021(3)	177.5
O12-H12C...O6	0.85	1.98	2.820(3)	170.6
O12-H12D...O9#1	0.85	2.00	2.844(3)	171.0
O13-H13C...O4	0.85	1.97	2.818(3)	179.7
O13-H13D...O12#1	0.85	2.04	2.892(3)	179.6
Complex <b>2</b> <sup>a</sup>				
O7-H7...O9	0.82	1.90	2.718(3)	175.4
O8-H8A...O7	0.85	1.96	2.807(3)	172.9
O8-H8B...O10#1	0.85	2.07	2.915(4)	173.2
O9-H9A...O10	0.85	2.15	2.985(4)	169.6
O9-H9B...O11	0.85	1.98	2.819(4)	170.1
O10-H10A...O4#2	0.85	1.98	2.831(3)	176.0
O10-H10B...O13#1	0.85	1.93	2.777(4)	176.2
O11-H11C...O12	0.85	1.83	2.681(3)	176.7
O11-H11D...N8#2	0.85	2.17	3.015(3)	176.8
O12-H12A...N2#3	0.85	1.96	2.741(4)	152.5
O13-H13A...O1#4	0.85	1.90	2.745(4)	171.7
O13-H13B...O8#1	0.85	2.04	2.886(4)	172.1
O15-H15A...O2#4	0.85	2.10	2.909(3)	158.9

<sup>a</sup>Symmetry transformations used to generate equivalent atoms for **1**: #1  $-x + 1, -y + 1, -z + 1$ ; #2  $-x + 1, -y + 2, -z + 1$ ; #3  $x - 1, y, z$ ; for **2**: #1  $-x + 1, -y + 1, -z + 1$ ; #2  $x + 1, y, z$ ; #3  $-x + 1, -y, -z + 1$ ; #4  $-x, -y + 1, -z + 1$ .

is 10.050 Å. The 1D tubular structure is filled by the large crystallographically unique uncoordinated water molecules involved in strong O—H...O and O—H...N hydrogen bonds (Fig. 3 and Table 3). However, to our knowledge, the 1D tubular structure with so many uncoordinated water molecules is seldom.

Actually, the results of X-ray crystallographic analysis revealed that complex **2** is also a 1D tubular structure that is great similar to complex **1** except that the IPA<sup>2+</sup> is replaced by OH-BDC<sup>2+</sup> (Fig. 4). The complex **2** crystallizes in the triclinic space group *P*<sub>1</sub>. The Zn metal centers of complex **2** are six-coordinated by three carboxylate oxygen atoms (O4, O5, and O2B) from two OH-BDC<sup>2+</sup>, and three nitrogen atoms (N1, N7, and N12A) from three fluconazoles. The bond distances of Zn—O and Zn—N are in the range of 2.051(2)–2.3613(18) and 2.120(2)–2.148(2). The Zn—Zn distance connected two adjacent zinc atoms by OH-BDC<sup>2+</sup> ligands is 10.083 Å and the Zn—Zn distance connected two

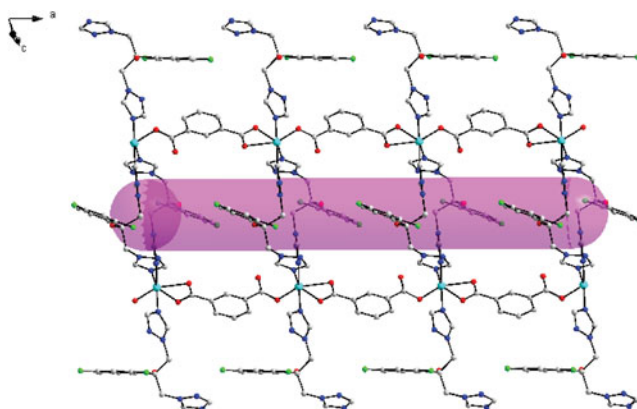


**Figure 1.** (a) Coordination environment of Zn(II) ions in **1** with thermal ellipsoids at 30% probability (hydrogen atoms were omitted for clarity). Symmetry code: (A)  $1+x, y, z$ ; (B)  $2-x, 1-y, 1-z$ . (b) Distorted rectangular cavity in **1**.

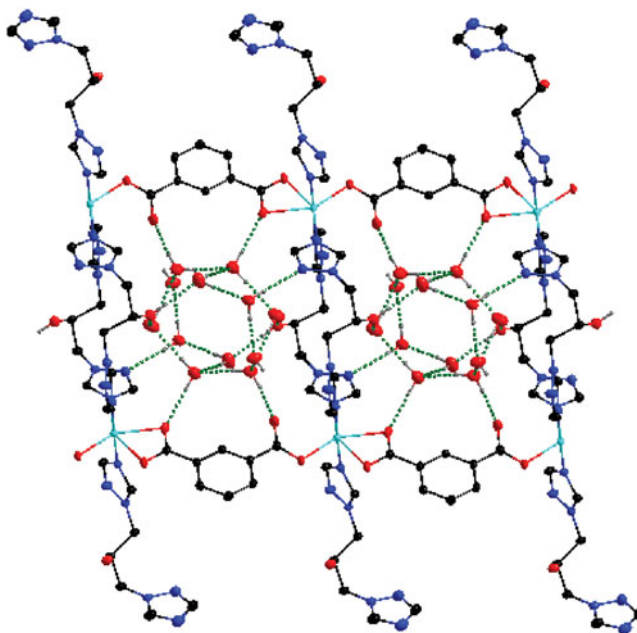
adjacent zinc atoms by fluconazole ligands is  $10.402 \text{ \AA}$ . All these values are comparable to those of complex **1**. The size of the distorted dinuclear zinc rectangular-shaped cavity  $[\text{Zn}(1)\text{-C}(24)\text{-Zn}(1\text{A})\text{-C}(24\text{A})]$  in complex **2** is  $5.659 \times 7.887$  (Fig. 5(a)). Each carboxylate group of the  $\text{OH-H}_2\text{BDC}$  ligands is completely deprotonated, and the two completely deprotonated carboxylate group adopts bidentate chelating and monodentate coordination modes as well (Fig. 4(b)). The hydroxyl group ( $-\text{OH}$ ) of  $\text{OH-H}_2\text{BDC}$  neither takes part in coordination nor is involved in weak interactions to metal centers. Large free water molecules involved in strong  $\text{O-H}\cdots\text{O}$  and  $\text{O-H}\cdots\text{N}$  hydrogen bonds are accommodated in the residual empties and further stabilize the structural framework (Fig. 5(b) and Table 3).

### Infrared Spectroscopy

The IR spectrum of compound **1** displays characteristic bands of carboxyl groups at  $1616 \text{ cm}^{-1}$  and  $1540 \text{ cm}^{-1}$  for the antisymmetric stretching and at  $1418 \text{ cm}^{-1}$  and  $1373 \text{ cm}^{-1}$



**Figure 2.** The 1D tubular structure in **1**.



**Figure 3.** A perspective view of uncoordinated crystallization water molecules and selected hydrogen bonds lying inside the one-dimensional tubes in **1** (phenyl groups of HFlu are omitted for clarity).

for symmetric stretching. For **2**, the characteristic bands of the carboxylate groups are shown at  $1617\text{ cm}^{-1}$  and  $1575\text{ cm}^{-1}$  for asymmetric and at  $1419\text{ cm}^{-1}$  and  $1376\text{ cm}^{-1}$  for symmetric vibrations, respectively. The separations ( $\Delta$ ) between  $\nu_{\text{asym}}(\text{CO}_2)$  and  $\nu_{\text{sym}}(\text{CO}_2)$  bands show that the carboxylate groups coordinate to the metal atoms. The absence of the characteristic bands at around  $1700\text{ cm}^{-1}$  in compounds **1** and **2** indicates the complete deprotonation of carboxylic groups [25].

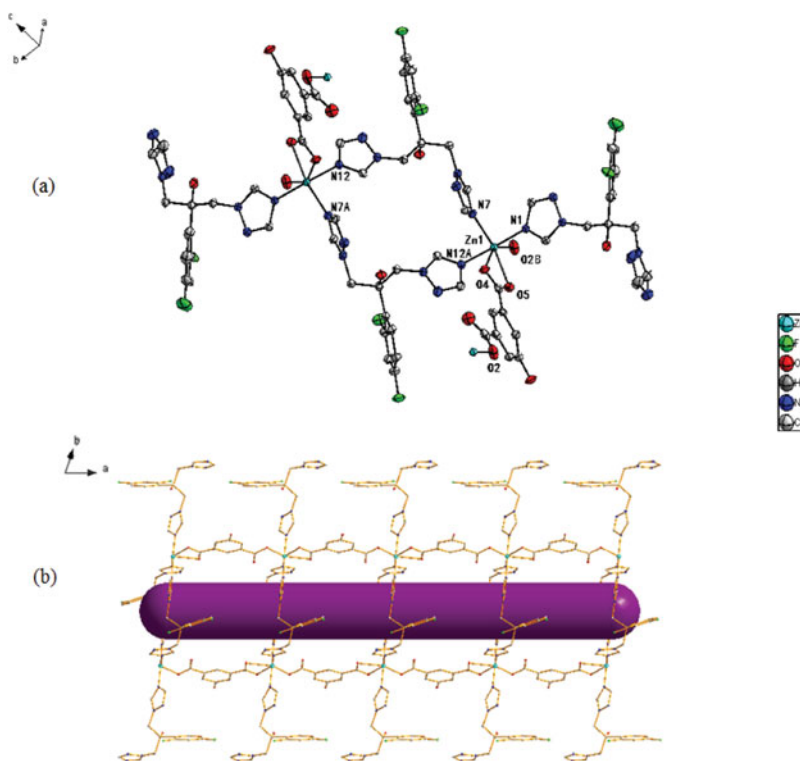
### Fluorescence Properties

Coordination complexes, especially with  $d^{10}$  metal centers, have been investigated for fluorescence properties owing to their potential applications as luminescent materials. Therefore, in the present study, the photoluminescence properties of **1** and **2** as well as free fluconazole ligand were investigated in the solid state at room temperature and the results were shown in Fig. 6. Under the 253 nm excitation, the fluconazole ligand emits strongly at 302 nm assigned to the  $\pi^* \rightarrow \pi$  transition. Complex **1** gives fluorescence at 339 nm under 248 nm and complex **2** gives relatively weak fluorescence at 390 nm under 245 nm. However, Compared with the free ligand (HFlu), the fluorescence emissions of **2** exhibit quenching phenomenon. The emission bands of compounds **1** and **2** exhibit redshift, which probably results from the metal coordination as well as the introduction of  $\text{IPA}^{2-}$  ligand and  $\text{OH-BDC}^{2+}$  ligand.

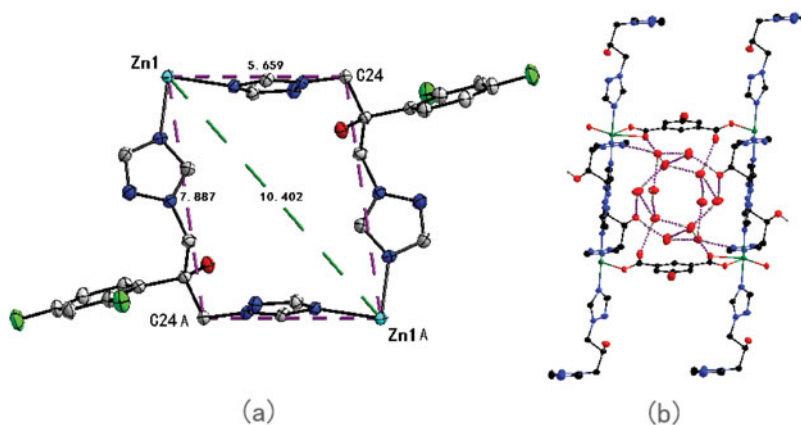
### Thermal Properties

TGA of complex **1** and **2** under the nitrogen atmosphere was performed to study the thermal stability. As shown in Fig. 7, complex **1** displays the first weight loss of 17.1% in

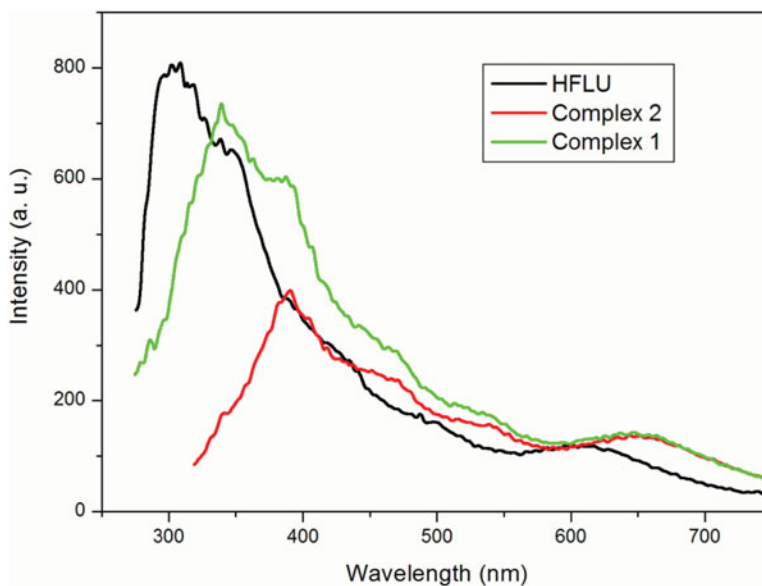




**Figure 4.** (a) Coordination environment of Zn(II) ions in **2** with thermal ellipsoids at 30% probability (hydrogen atoms were omitted for clarity). Symmetry code: (A)  $-x, 1-y, 1-z$ ; (B)  $1+x, y, z$ . (b) The 1D tubular structure in **2**.

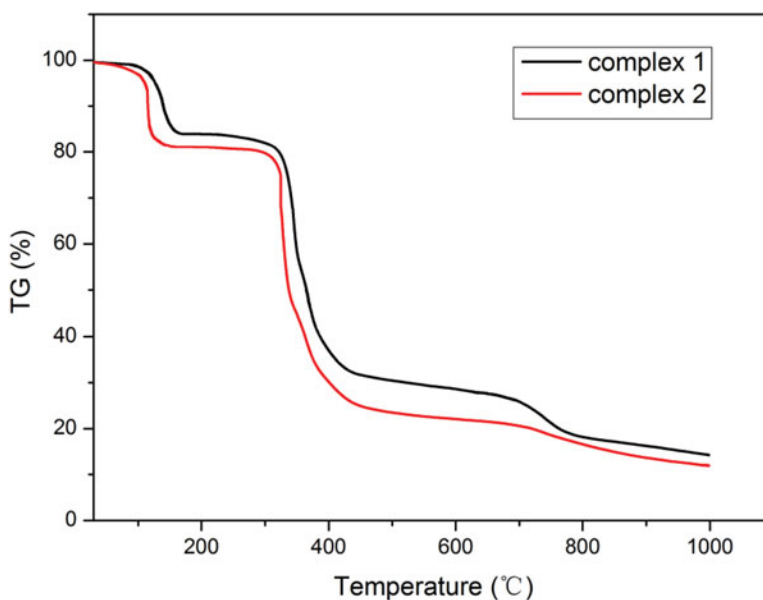


**Figure 5.** (a) Distorted rectangular cavity in **2**. (b) A perspective view of uncoordinated crystallization water molecules and selected hydrogen bonds lying inside the one-dimensional tubes in **2** (phenyl groups of HFlu are omitted for clarity).



**Figure 6.** Emission spectra for **1**, **2** and HFLu in the solid state at room temperature.

the temperature range of 50°C–145°C, corresponding to the loss of lattice water molecules (calcd.: 16.2%). Continuous heating brought about the pyrolysis of HFLu ligand and IPA<sup>2-</sup> ligand until 1000°C. For **2**, the weight loss of 16.0% before 171°C can be attributed to the loss of lattice water molecules (calcd.: 15.5%). Further heating led to a sharp weight loss and a rapid framework decomposition.



**Figure 7.** The TGA curves for **1** and **2**.

## Conclusion

In summary, based on fluconazole ligand, two zinc coordination polymers have been synthesized. X-ray analysis revealed complex **1** and **2** are both a tubular structure with the distorted dinuclear zinc rectangular-shaped cavity, and large free water molecules are accommodated in the 1D tubular structure. To our knowledge, the 1D tubular structure with so many uncoordinated water molecules is seldom. The thermal stability and fluorescent property of complexes **1** and **2** have also been studied. The work may provide helpful information for the design and construction of 1D tubular structure.

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## Supplementary Material

CCDC-957315 and CCDC-957316 contain the supplementary crystallographic data for complexes **1** and **2**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

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