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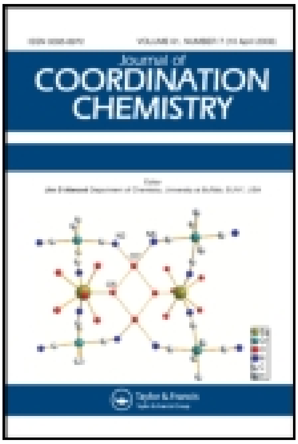

Journal of Coordination Chemistry
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gcoo20

Hydrothermal syntheses and crystal structures of two Zn(II) complexes with 1-substituted-1H-[1,2,3]-triazole-4-carboxylic acid

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Published online: 09 Aug 2011.

To cite this article: Hong Zhao, Jin-Mei Chen, Jin-Rui Lin & Wen-Xiang Wang (2011) Hydrothermal syntheses and crystal structures of two Zn(II) complexes with 1-substituted-1H-[1,2,3]-triazole-4-carboxylic acid, Journal of Coordination Chemistry, 64:15, 2735-2745, DOI: 10.1080/00958972.2011.606365

To link to this article: http://dx.doi.org/10.1080/00958972.2011.606365

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Journal of Coordination Chemistry
Vol. 64, No. 15, 10 August 2011, 2735–2745

Hydrothermal syntheses and crystal structures of two Zn(II) complexes with 1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acid

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(*Received 13 September 2010; in final form 24 June 2011*)

Two new Zn(II) complexes, $[Zn(L)_2(H_2O)_2]$ where L is 1-substituted 5-methyl-1*H*-[1,2,3]-triazole-4-carboxylic acid, have been synthesized and characterized by elemental analysis, FT–IR, and solid-state fluorescent emission spectroscopy. Structures have been established by single-crystal X-ray diffraction, revealing the discrete nature of the complexes in which Zn centers adopt slightly distorted octahedral geometry. In the complexes, the 1-substituted 5-methyl-1*H*-[1,2,3]-triazole-4-carboxylic acid is bidentate.

Keywords: Zinc(II) complex; Hydrothermal synthesis; Triazole

1. Introduction

Crystal engineering strategies attempt to predict and control crystal packing arrangements with desired symmetry that will provide a physical property of interest. Since the structural diversity of coordination polymers mainly comes from the geometry and topology of ligands, many ligands are synthesized and intensively investigated for supramolecular architecture. Of the many organic ligands investigated, heterocyclic carboxylic acids such as pyridine-, pyrazole-, and triazole-carboxylic acids constitute an important family [1–12]. These acids can act as multiple proton donors and acceptors and use their carboxylate and nitrogens to coordinate metal ions, forming interesting network structures.

1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acid derivatives [13–16] exhibit antimicrobial activity, as inhibitors of human leukocyte elastase, as synthons for the preparation of antitumor dehydropyrrolizidine alkaloids, and for modification of nucleosides as antiviral agents. Recently, Zheng *et al.* [17] synthesized four transition metal complexes with the *in situ* formation of unsubstituted [1,2,3]-triazole-4-carboxylate. Few coordination compounds with 1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acid have been found [18]. We report the synthesis, elemental analyses,

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Journal of Coordination Chemistry
ISSN 0095-8972 print/ISSN 1029-0389 online © 2011 Taylor & Francis
DOI: 10.1080/00958972.2011.606365

spectroscopic studies, and crystal structures of two new mononuclear Zn(II) complexes with 1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acid to obtain a deeper insight into the application of 1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acids in crystal engineering as multi-functional ligands.

2. Experimental

2.1. *Reagents and measurements*

All chemicals and solvents were commercially available and used without purification. Elemental analyses for carbon, hydrogen, and nitrogen were performed on a Perkin Elmer 240C elemental analyzer. IR spectra were obtained with KBr pellets from 4000 to 400 cm^{-1} using a Shimadzu IRprestige-21 spectrophotometer. ^{1}H-NMR and ^{13}C-NMR spectra were acquired on a Bruker 300 MHz spectrometer. The crystal structures were determined on a Rigaku SCX mini diffractometer. Luminescence spectra for the solid samples were investigated with a Shimadzu RF-5301pc fluorescence spectrophotometer.

2.2. *Synthesis of the complexes*

2.2.1. Synthesis of 1-(4-iodophenyl)-5-methyl-1*H*-[1,2,3]-triazole-4-carboxylic acid (HL^1). To 4-iodobenzenamine (2.19 g, 10 mmol) in concentrated HCl (3.3 mL) and water (10 mL), $NaNO_2$ (0.69 g, 10 mmol) in water (5 mL) was added at 0–5°C. The mixture was stirred at 0°C for 1 h and then filtered. To the filtrate, NaN_3 (0.65 g, 10 mmol) in water (5 mL) was added dropwise. The reaction mixture was stirred at 0°C for 1 h, then extracted with Et_2O (3×50 mL), and the combined organic layers were washed with water and dried (Na_2SO_4) and the solvent was removed under vacuum. To the resulting residue, ethyl 3-oxobutanoate (1.43 g, 11 mmol) was added. Then, NaOEt (1.02 g, 15 mmol) in EtOH (100 mL) was added dropwise to the mixture at 0°C. After addition, the mixture was heated at 90°C for 8 h and then cooled to room temperature. To the reaction mixture, concentrated HCl at $pH \approx 1$ was added. The white precipitate was collected and washed with water to give the crude product. HL^1 was obtained (2.05 g, 70.5%) after recrystallization from ethanol (95%); IR (KBr; cm^{-1}): 3050(w), 1690(vs), 1559(vs), 1492(vs), 1448(s), 1392(m), 1272(s), 1122(m), 990(s), 926(m), 883(m), 802(m), 782(m), and 509(m). ^{1}H-NMR (DMSO-d_6): δ 13.17 (br, s, 1H, COOH), 7.98 (d, 2H, $J = 6.4$ Hz, phenyl), 7.43 (d, 2H, $J = 7.83$ Hz, phenyl), and 2.58 (s, 3H, CH_3); ^{13}C-NMR (DMSO-d_6): δ 162.9, 139.3, 138.9, 137.1, 135.4, 127.6, 96.7, and 10.27 ppm.

2.2.2. Synthesis of 5-methyl-1-(4-nitrobenzyl)-1*H*-[1,2,3]-triazole-4-carboxylic acid (HL^2). To 1-methyl-3-nitrobenzene (2.74 g, 20 mmol) in CCl_4 (100 mL), N-bromosuccinimide (3.56 g, 20 mmol) and benzoyl peroxide (0.2 g) were added. The mixture was heated at 90°C for 20 h and then cooled and filtered. The filtrate was concentrated to 40 mL and 1-(bromomethyl)-3-nitrobenzene (3.54 g, 82.5%) was collected by filtration and recrystallized in EtOH. A mixture of 1-(bromomethyl)-3-nitrobenzene (2.15 g, 10 mmol) and NaN_3 (0.98 g, 15 mmol) in CH_3CN (80 mL) was heated under reflux for

24 h, and then cooled and filtered. The solvent was removed under vacuum to give 1-(azidomethyl)-3-nitrobenzene, which was used without purification. To the residue, ethyl 3-oxobutanoate (1.43 g, 11 mmol) was added. Then, NaOEt (1.02 g, 15 mmol) in EtOH (100 mL) was added dropwise to the mixture at 0°C. After addition, the mixture was heated at 90°C for 8 h and then cooled to room temperature. To the reaction mixture, concentrated HCl at $pH \approx 1$ was added. The white precipitate was collected and washed with water to give crude HL^2 (1.73 g, 70%); it was used without further purification after recrystallization from ethanol (95%). IR (KBr; cm^{-1}): 3150(w), 1695(vs), 1588(m), 1534(vs), 1480(m), 1356(vs), 1265(m), 1250(s), 1218(s), 1096(m), 988(m), 903(m), 805(m), 735(m), and 557(m). ^{1}H-NMR (DMSO-d_6): δ 13.42 (br, s, 1H, COOH), 8.15 (m, 2H, phenyl), 7.66 (m, 2H, phenyl), 5.79 (s, 2H, CH_2), and 2.61 (s, 3H, CH_3); ^{13}C-NMR (DMSO-d_6): δ 162.9, 148.1, 139.1, 137.3, 137.1, 134.3, 130.6, 123.2, 122.5, 50.29, and 8.96 ppm.

2.2.3. Synthesis of $[ZnL^1_2(H_2O)_2]$ (1). $ZnCl_2$ (0.136 g, 1 mmol) and HL_1 (0.658 g, 2 mmol) were placed in a thick Pyrex tube (*ca* 20 cm in length). After the addition of 2.0 mL of water, the tube was frozen with liquid N_2, evacuated, and sealed with a torch. The tube was heated at 120°C for 2 days to give colorless prism crystals (pure phase) in 68% yield based on $ZnCl_2$. IR (KBr; cm^{-1}): 3443(w), 1625(s), 1600(s), 1496(m), 1428(s), 1377(m), 1313(s), 1300(m), 1242(m), 1141(m), 1014(w), 831(m), and 765(m). Anal. Calcd for $C_{20}H_{18}I_2N_6O_6Zn$ (%): C, 33.71; H, 2.39; and N, 11.09. Found (%): C, 33.67; H, 2.35; and N, 11.12.

2.2.4. Synthesis of $[ZnL^2_2(H_2O)_2]$ (2). $ZnCl_2$ (0.136 g, 1 mmol) and HL_2 (0.524 g, 2 mmol) were placed in a thick Pyrex tube (*ca* 20 cm in length). After the addition of 2.0 mL of water, the tube was frozen with liquid N_2, evacuated, and sealed with a torch. The tube was heated at 120°C for 3 days to give colorless block crystals (pure phase) in 54% yield based on $ZnCl_2$. IR (KBr; cm^{-1}): 3377(w), 1620(s), 1615(s), 1581(s), 1556(m), 1496(m), 1421(m), 1392(s), 1377(m), 1313(w), 1292(w), 1246(w), 1138(m), 1074(m), 1016(m), 835(m), and 769(m). Anal. Calcd for $C_{22}H_{22}N_8O_{10}Zn$ (%): C, 42.36; H, 3.55; and N, 17.96. Found (%): C, 42.29; H, 3.49; and N, 17.89.

2.3. *X-ray crystal structure determination*

X-ray diffraction data of **1** and **2** were collected on a Rigaku SCX mini diffractometer using Mo-Kα radiation ($\lambda = 0.71073$ Å). The structure was solved by direct methods with SHELXS-97 and refined by full matrix least squares on F^2 with SHELXL-97 [19]. All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogens were added theoretically and refined with a riding model and fixed isotropic thermal parameters. Detailed data collection and refinements of **1** and **2** are summarized in table 1. Selected bond lengths and angles are listed in table 2. Relevant hydrogen-bonding parameters of **1** and **2** are summarized in table 3.

Table 1. Crystallographic data and structure refinement parameters for **1** and **2**.

	1	**2**
Empirical formula	$C_{20}H_{18}I_2N_6O_6Zn$	$C_{22}H_{22}N_8O_{10}Zn$
Formula weight	757.59	623.85
Temperature (K)	293(2)	293(2)
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/n$	$P\bar{1}$
Unit cell dimensions (Å, °)		
a	7.0965(14)	6.6360(10)
b	26.915(5)	9.0470(15)
c	7.1388(14)	11.409(2)
α	90.00	97.905(7)
β	115.37(3)	97.770(7)
γ	90.00	110.188(16)
Volume (Å^3), Z	1232.0(5), 2	624.35(18), 1
Calculated density (g cm^{-3})	2.042	1.659
Absorption coefficient (mm^{-1})	3.551	1.058
$F(000)$	728	320
Crystal size (mm^3)	0.18 × 0.20 × 0.25	0.12 × 0.18 × 0.20
θ range for data collection (°)	3.03–27.48	2.75–27.46
Reflections collected	12,716	6372
Independent reflection	2824	2816
Goodness-of-fit on F^2	1.106	1.175
Final R indices $[I>2\sigma(I)]$	$R_1=0.0388$, $wR_2=0.0757$	$R_1=0.0297$, $wR_2=0.0820$
R indices (all data)	$R_1=0.0524$, $wR_2=0.0804$	$R_1=0.0335$, $wR_2=0.0953$
Largest difference peak and hole (e Å^{-3})	0.563 and −0.848	0.458 and −0.359

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

3. Results and discussion

3.1. *Complexes synthesis*

Complex **1** was synthesized hydrothermally by treating $ZnCl_2$ and HL_1 at 120°C, while **2** was obtained by treating $ZnCl_2$ and HL_2 at the same conditions (scheme 1).

3.2. *Structural description of 1 and 2*

3.2.1. $[ZnL^1_2(H_2O)_2]$ (1). The crystal structure of **1** shows that each asymmetric unit contains one L_1, one Zn, and one water molecule. The local coordination geometry around Zn can be described as a slightly distorted octahedron (figure 1). The Zn coordinates to two water molecules with a Zn–O distance of 2.086(2) Å in the axial positions and to two carboxylate oxygens and two triazole nitrogens of two L_1 ligands in a *trans* fashion with a Zn–O distance 2.070(2) Å and a Zn–N distance 2.189(3) Å. The O_1–Zn–O_1A angle is 180.00(12)°, whereas the N–Zn–O angles around the Zn center range from 78.63(10) to 101.37(10)°. In **1**, the deprotonated HL_1 is bidentate with one oxygen of carboxylate and one nitrogen of 1,2,3-triazole ring chelating to Zn, resulting in the formation of a stable five-numbered ring (Zn_1–O_1–C_1–C_2–O_3). In the crystal packing of **1**, the uncoordinated O_2 of carboxylate forms a strong hydrogen bond (2.712(2) and 2.725(2) Å) with the coordinated water molecule, resulting in a 2-D network in the *ac*-plane (figure 2). In the 2-D network, the Zn–Zn distances through

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

1[a]			
Zn(1)–O(1)	2.070(2)	Zn(1)–O(1)$^{\#1}$	2.070(2)
Zn(1)–O(3W)	2.086(2)	Zn(1)–O(3W)$^{\#1}$	2.086(2)
Zn(1)–N(3)$^{\#1}$	2.189(3)	Zn(1)–N(3)	2.189(3)
C(1)–O(2)	1.251(4)	C(1)–O(1)	1.257(4)
C(1)–C(2)	1.485(5)	C(2)–N(3)	1.360(4)
C(2)–C(3)	1.381(5)	C(3)–N(1)	1.348(5)
C(3)–C(4)	1.495(4)	N(1)–N(2)	1.368(4)
N(2)–N(3)	1.297(4)	C(8)–I(1)	2.091(4)
O(1)–Zn(1)–O(1)$^{\#1}$	180.00(12)	O(1)–Zn(1)–O(3W)	88.27(9)
O(1)$^{\#1}$–Zn(1)–O(3W)	91.73(9)	O(1)–Zn(1)–O(3W)$^{\#1}$	91.73(9)
O(1)$^{\#1}$–Zn(1)–O(3W)$^{\#1}$	88.27(9)	O(3W)–Zn(1)–O(3W)$^{\#1}$	180.00(12)
O(1)–Zn(1)–N(3)$^{\#1}$	101.37(10)	O(1)$^{\#1}$–Zn(1)–N(3)$^{\#1}$	78.63(10)
O(3W)–Zn(1)–N(3)$^{\#1}$	86.44(10)	O(3W)$^{\#1}$–Zn(1)–N(3)$^{\#1}$	93.56(10)
O(1)–Zn(1)–N(3)	78.63(10)	O(1)$^{\#1}$–Zn(1)–N(3)	101.37(10)
O(3W)–Zn(1)–N(3)	93.56(10)	O(3W)$^{\#1}$–Zn(1)–N(3)	86.44(10)
N(3)$^{\#1}$–Zn(1)–N(3)	180.00(12)		
2[b]			
Zn(1)–O(1)$^{\#1}$	2.0719(14)	Zn(1)–O(1)	2.0719(14)
Zn(1)–N(1)$^{\#1}$	2.1253(15)	Zn(1)–N(1)	2.1253(15)
Zn(1)–O(1W)$^{\#1}$	2.1611(14)	Zn(1)–O(1W)	2.1611(14)
C(1)–O(2)	1.234(2)	C(1)–O(1)	1.268(2)
C(1)–C(2)	1.494(2)	C(2)–C(3)	1.368(2)
C(2)–N(1)	1.353(2)	C(3)–N(3)	1.351(2)
C(3)–C(4)	1.491(3)	N(1)–N(2)	1.306(2)
N(2)–N(3)	1.350(2)		
O(1)$^{\#1}$–Zn(1)–O(1)	180.00(1)	O(1)$^{\#1}$–Zn(1)–N(1)$^{\#1}$	78.85(5)
O(1)–Zn(1)–N(1)$^{\#1}$	101.15(5)	O(1)$^{\#1}$–Zn(1)–N(1)	101.15(5)
O(1)–Zn(1)–N(1)	78.85(6)	N(1)$^{\#1}$–Zn(1)–N(1)	180.00(1)
O(1)$^{\#1}$–Zn(1)–O(1W)$^{\#1}$	85.58(5)	O(1)–Zn(1)–O(1W)$^{\#1}$	94.42(5)
N(1)$^{\#1}$–Zn(1)–O(1W)	88.96(6)	N(1)–Zn(1)–O(1W)$^{\#1}$	91.04(6)
O(1)$^{\#1}$–Zn(1)–O(1W)	94.42(5)	O(1)–Zn(1)–O(1W)	85.58(5)
N(1)$^{\#1}$–Zn(1)–O(1W)	91.04(6)	N(1)–Zn(1)–O(1W)	88.96(6)
O(1W)$^{\#1}$–Zn(1)–O(1W)	180.00(1)		

[a] Symmetry transformations used to generate equivalent atoms: $^{\#1}$ $2-x$, $1-y$, $-z$.
[b] Symmetry transformations used to generate equivalent atoms: $^{\#1}$A: $2-x$, $3-y$, $1-z$

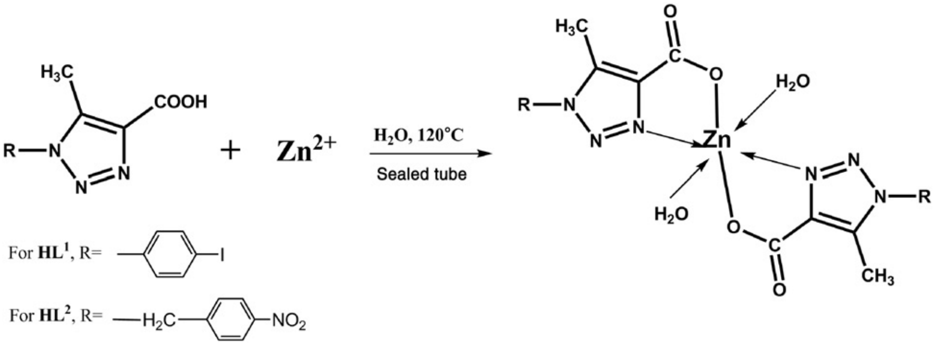
Table 3. Geometrical parameters of hydrogen bonds in **1** and **2**.

Compound	D–H···A	D–H (Å)	H···A (Å)	∠DHA (°)	D···A (Å)	Symmetry code of O
1	O3W–H3F···O2	0.768	1.974	161.18	2.712	$x+1$, y, z
	O3W–H3E···O2	0.956	1.775	172.00	2.725	$2-x$, $1-y$, $1-z$
2	O1W–H1F···O2	0.820	1.848	174.29	2.665	$1-x$, $3-y$, $1-z$
	O1W–H1E···O4	0.819	2.214	167.81	3.020	$2-x$, $2-y$, $1-z$

intermolecular hydrogen bonding are 7.096(1), 7.139(1), and 7.61(18) Å, respectively. As shown in figure 3, adjacent layers in **1** stack *via* π–π stacking interactions of phenyl rings with a centroid-to-centroid distance of 3.858(2) Å. No solvent molecules are enclathrated in **1**.

3.2.2. $[ZnL^2_2(H_2O)^2]$ (2).

Complex **2** is isostructural with **1** except that the coordinated L_1 are replaced by L_2. The Zn in **2** possesses a slightly distorted octahedral geometry



Scheme 1. Synthesis of complexes **1** and **2**.

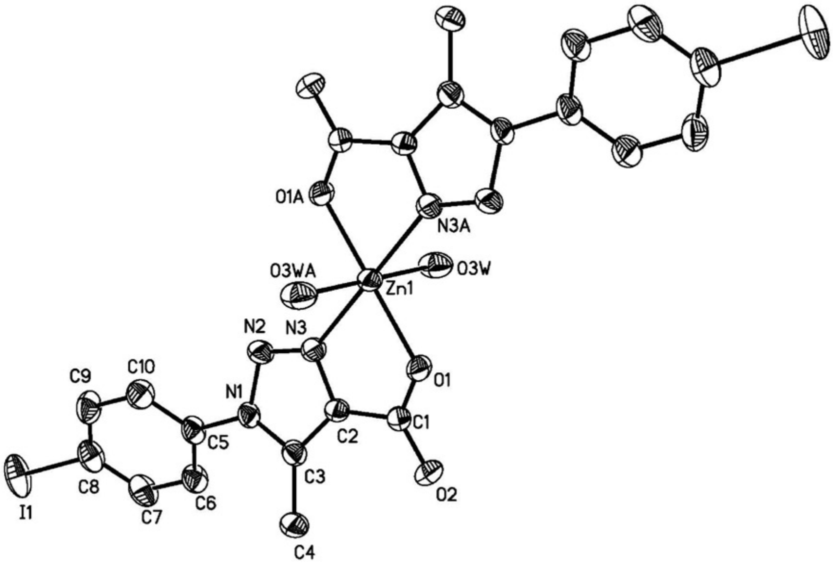


Figure 1. View of **1**, with atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level; hydrogens are omitted for clarity.

with its equatorial sites occupied by two carboxylate oxygens and two triazole nitrogens of two L_2 and its axial positions are occupied by two water molecules (figure 4). The Zn centers also form a 2-D network through hydrogen bonding with $O_1W–H_1F \cdots O_2$ and $O_1W–H_1E \cdots O_4$ (figure 5). The π–π stacking interactions are between adjacent triazole and phenyl rings with centroid-to-centroid distances of 4.163(1) and 4.624(1) Å, respectively.

3.3. *Characterizations of the complexes*

3.3.1. IR spectra. Broad bands at $3400\,\mathrm{cm}^{-1}$ suggest that coordination waters are present [20]. Neither **1** nor **2** shows any strong bands at *ca* $1700\,\mathrm{cm}^{-1}$, suggesting that

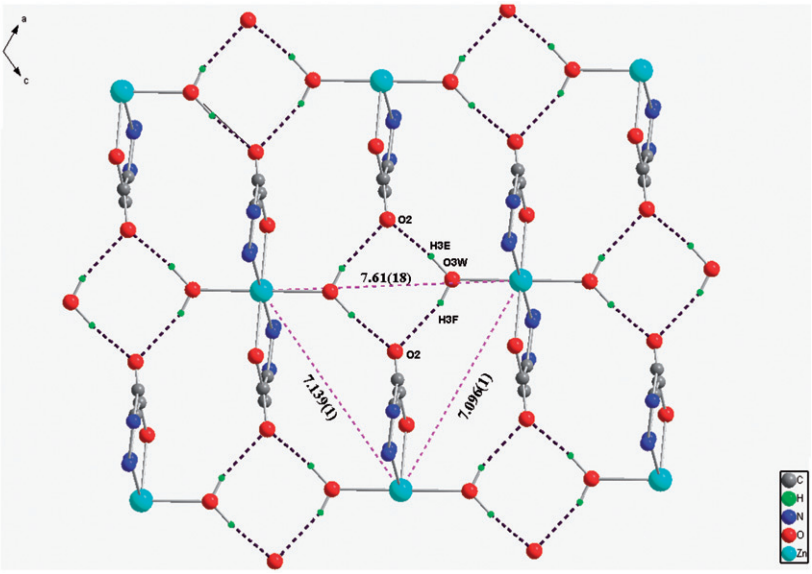


Figure 2. Hydrogen bonds formed in **1**. Aryl groups and methyl groups are omitted for clarity.

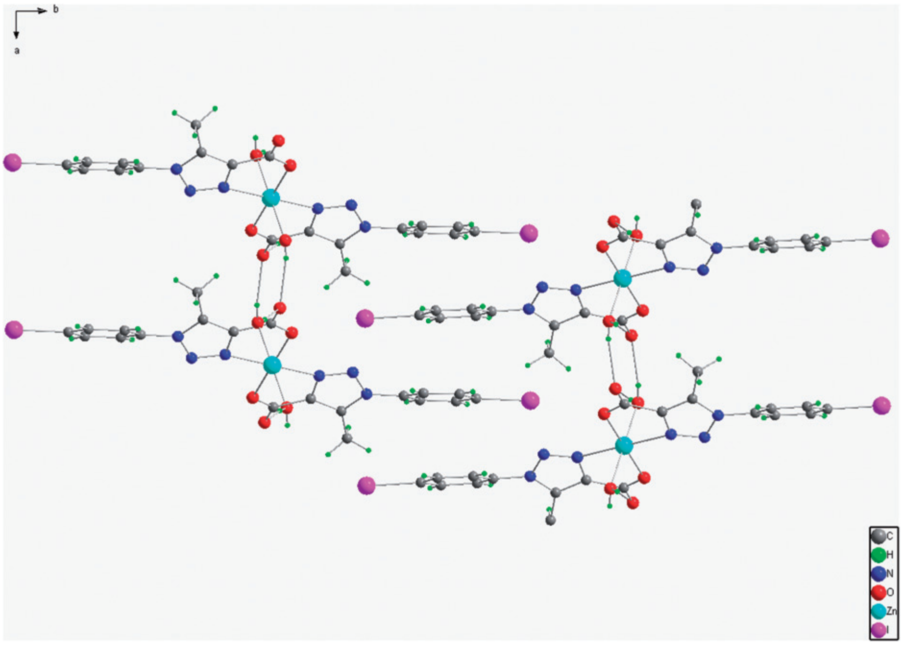


Figure 3. Adjacent 2-D layers in **1** as viewed along the *c*-axis. The π–π stacks formed between the phenyl rings are clearly visible.

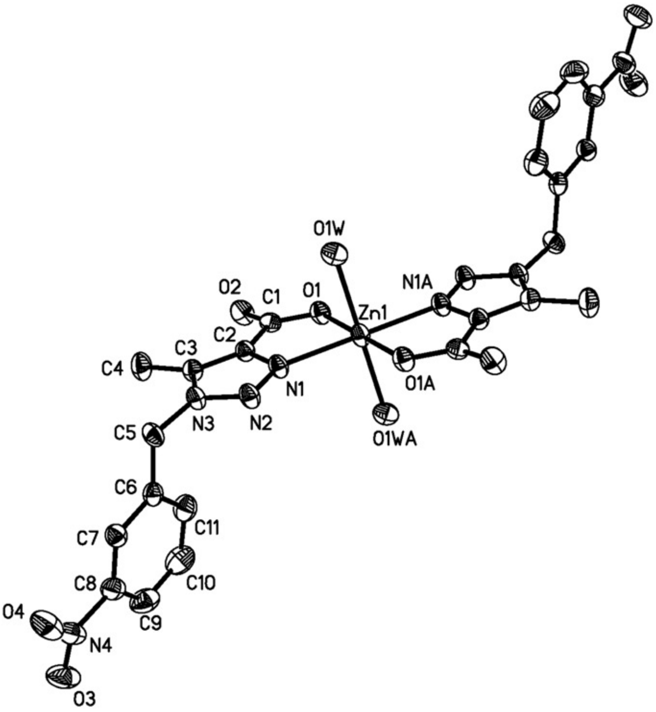


Figure 4. View of **2**, with atom number scheme. Displacement ellipsoids are drawn at the 30% probability level; hydrogens are omitted for clarity.

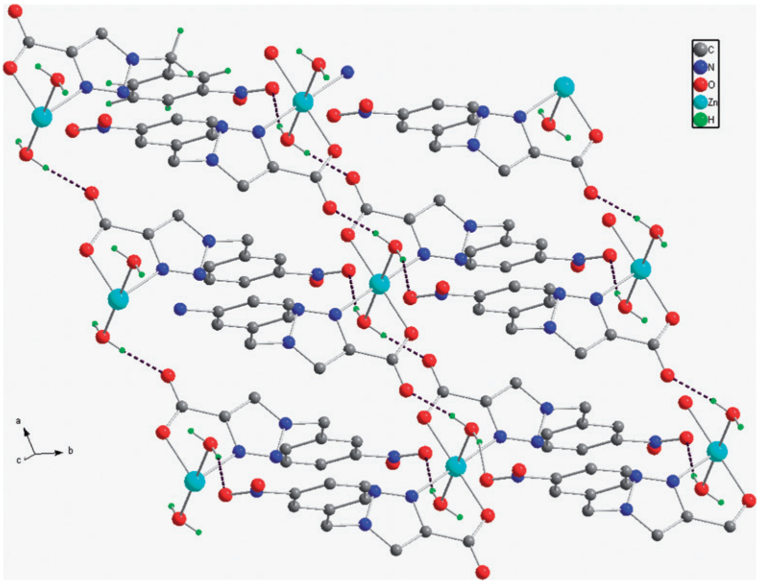


Figure 5. Hydrogen bonds formed in **2**. Methyl groups and some hydrogens are omitted for clarity.

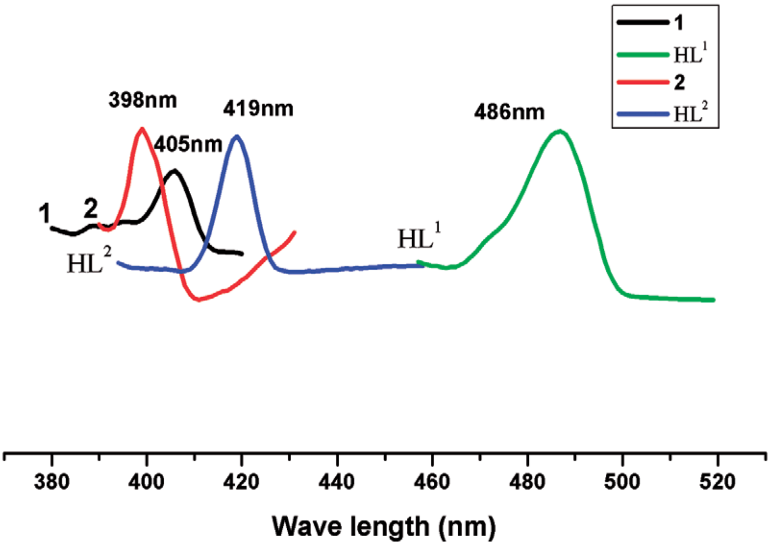


Figure 6. The solid-state photoluminescence spectra of **1**, **2** and the free ligands at room temperature.

both HL_1 and HL_2 are deprotonated in the complexes. Strong bands at 1600 and 1581 cm^{-1} in **1** and **2** may be attributed to the asymmetric stretching (ν_{as}) mode of the carboxylate group and bands at 1373 and 1377 cm^{-1} represent the symmetric stretching (ν_s) mode of this group. The corresponding difference between ν_{as} and ν_s are 227 for **1** and 204 for **2**, indicating the presence of monodentate carboxylate [20]. Bands at 1625 and 1428 cm^{-1} for **1** and 1615 and 1421 cm^{-1} for **2** strongly support the existence of coordinated N-donors arising from $\nu_{C=N}$ [21]. These conclusions are also supported by X-ray diffraction measurements.

3.3.2. Luminescent emission spectra. Coordination compounds, especially d^{10}-metals, have luminescent properties and potential application as photoactive materials [22–26]. The luminescence of **1** and **2** as well as the free ligands was investigated in the solid state at room temperature (figure 6). The luminescence spectrum of HL^1 shows emission at $\lambda_{max} = 486$ nm upon excitation at 350 nm and $\lambda_{max} = 419$ nm for HL^2 ligand ($\lambda_{ex} = 350$ nm). Complexes **1** and **2** exhibit an intense luminescence emission peak at 405 nm for **1** and $\lambda_{max} = 398$ nm for **2** ($\lambda_{ex} = 350$ nm). In comparison with the ligands, the emissions of **1** and **2** may be assigned to intraligand (π–π*) fluorescence [27–29]. Both **1** and **2** show purple fluorescent emission and may be used as fluorescent material for purple-light emitting diode devices.

4. Conclusions

We have synthesized and characterized two new 1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acid ligands and their Zn(II) complexes. Although many Zn(II) complexes containing triazole ligands have been found in the recent literature [30–34], in which most contain [1,2,4]-triazole derivatives, the Zn(II) complexes derived from 1-substituted 5-methyl-1*H*-[1,2,3]-triazole-4-carboxylic acid ligands are first reported. In the complexes, six coordination is completed in each complex by water molecules. The coordinated water molecules extend those complexes into 2-D structures by hydrogen bonds. Photoluminescent properties of 1-substituted-1*H*-[1,2,3]-triazole-4-carboxylic acid derivatives provide potential application of metal–organic complexes as photoluminescent materials.

Supplementary material

CCDC-775000 (**1**) and 777467 (**2**) contain the supplementary crystallographic data (excluding structure factor) for this article. These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: +44 1223 336 033; Email: deposit@ccdc.cam.ac.uk].

Acknowledgments

We gratefully acknowledge the financial support of the National Natural Science Foundation of China (20801012) and the financial support for Young researcher from Southeast University (4007041027).

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