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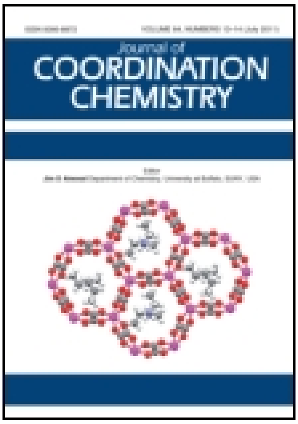

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Self-assembly of three supramolecular architectures based on an unsymmetrical N-heterocyclic ligand

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Three new compounds, $\{[Cd(Htmb)(Cl)(CH_3CO_2)] \cdot CH_3OH\}_n$ (**1**), $[Cd(Htmb)_2(Cl)_2(H_2O)_2] \cdot 4H_2O$ (**2**), and $[Cd(Htmb)_2(I)_2]$ (**3**) (Htmb = 2-(1H-triazol-1-ylmethyl)-1H-benzoimidazole), have been synthesized and characterized by elemental analysis, IR, and X-ray diffraction. Compound **1** features 1-D infinite double chains with space group $P\bar{1}$ and further forms a 3-D supramolecular structure by hydrogen bonds and π–π interactions. Compound **2** displays a mononuclear structure with space group $P2/c$, wherein an interesting water chain is formed. Compound **3** shows a mononuclear structure with space group $P2_1/n$ and extends into a 3-D supramolecular structure through hydrogen bonds and π–π interactions. In addition, the spectral properties are investigated, with strong luminescence observed for **1** and **2**.

Keywords: Cadmium compound; Crystal structure; Luminescence

1. Introduction

Supramolecular compounds have attracted attention for fascinating structures and potential applications in fluorescence, catalysis, magnetism, ion exchange, etc. Supramolecular architectures organized by coordinate covalent bonds occur between organic ligands with specific functional groups and metal ions with different binding preferences and/or weak non-covalent interactions, such as hydrogen bonds, aromatic stacking, van der Waals forces, etc. [1–7]. The preparation of supramolecular compounds from organic ligands and metal salts remains, however, a challenge [8]. In previous reports, synthetic strategies such as design of organic ligands, selection of metal salts, solvent systems, concentration, temperature, and pH are significant for the construction of novel structures and new materials [9, 10]. Consequently, reasonable design of organic ligands and control of reaction conditions are very important for constructing supramolecular compounds with interesting properties. Many compounds

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based on N-heterocyclic organic ligands, such as triazole, tetrazole, benzoimidazole, and derivatives have been reported; however, the investigation of unsymmetrical N-heterocyclic ligands is still rather limited [11]. Recently, Liu *et al.* [12] reported a silver polymer $[AgL]_n$ (HL = 1H-1,2,4-triazole-1-methylene-1H-benzoimidazole-1-acetic acid) that exhibits a 2-D layered structure. In addition, Wang *et al.* [13] described two polymers $[Cd_2(L)_4(\mu_2\text{-}X)(X)(H_2O)]_n$ [X = Cl (**1**) and Br (**2**)] [L = 2-(1H-imidazol-1-ylmethyl)-1H-benzoimidazole] that crystallized in noncentrosymmetric space group and showed second harmonic generation response and ferroelectric behavior.

We are exploring the design and preparation of supramolecular compounds based on unsymmetrical N-heterocyclic ligands. In this article, we report an unsymmetrical N-heterocyclic ligand: 2-(1H-triazol-1-ylmethyl)-1H-benzoimidazole) (Htmb) and three 3-D supramolecular architectures: $\{[Cd(Htmb)(Cl)(CH_3CO_2)]\cdot CH_3OH\}_n$ (**1**), $[Cd(Htmb)_2(Cl)_2(H_2O)_2]\cdot 4H_2O$ (**2**), and $[Cd(Htmb)_2(I)_2]$ (**3**). Compound **1** features a 1-D infinite chain while **2** and **3** display mononuclear structures. These compounds further form 3-D supramolecular structures by hydrogen bonds and π–π interactions. Solid state fluorescence spectra of free Htmb and **1**–**3** are investigated, with strong luminescence of **1** and **2** being found.

2. Experimental

2.1. *Materials and measurements*

All chemicals from commercial sources were of reagent grade and used without purification. Elemental analyses (C, H, and N) were performed on a Carlo-Erba 1160 Elemental analyzer. IR spectra were recorded from 4000 to 400 cm^{-1} on a Nicolet NEXUS 470-FTIR Spectrophotometer with pressed KBr pellets. ^1H NMR spectra were recorded on a Bruker AVANCE II 400 NMR spectrometer using DMSO-d_6 solution at room temperature. Emission spectra were taken using a F-4500 HITACHI fluorescence spectrophotometer.

2.2. *Synthesis of Htmb*

2-(1H-triazol-1-yl) acetic acid used as starting material was prepared according to the reported procedure [14] as follows: *o*-phenylenediamine (4.320 g, 40 mmol) and 2-(1H-triazol-1-yl) acetic acid (6.540 g, 40 mmol) were mixed. To the above mixture, 30 mL polyphosphoric acid was added. The mixture was stirred at 180°C. After 4 h, the mixture turned to green color. The mixture was then cooled to room temperature and neutralized with ammonia water. The crude product was isolated by filtration and then crystallized from water. Yield: 5.321 g (67%); m.p. 197–199°C. ^1H NMR (400 MHz, DMSO) dppm: 8.696 (s, –NH–, 1H), 8.008 (s, triazole, 1H), 7.832 (s, triazole, 1H), 7.146–7.537 (m, benzene, 4H), 5.67 (s, $-CH_2-$, 2H). IR (KBr, cm^{-1}): 3398(w), 3100(w), 2958(w), 2876(w), 1942(w), 1628(m), 1621(m), 1587(w), 1513(s), 1461(s), 1335(s), 1274(s), 1140(m), 1019(s), 848(m), 744(s), 677(m), 648(m).

2.3. *Synthesis of $\{[Cd(Htmb)(Cl)(CH_3CO_2)]\cdot CH_3OH\}_n$ (1)*

A solution of $Cd(Ac)_2\cdot 2H_2O$ (0.1 mmol 26.6 mg) in methanol (4 mL), KCl (0.1 mmol, 7.5 mg) water (2 mL), and Htmb (0.1 mmol, 19.9 mg) in methanol (4 mL) were mixed in a sealed Teflon-lined stainless steel vessel (25 mL) at 100°C for 5 days. After cooling to room temperature, colorless, rod-like crystals were obtained. Yield: 48% based on Cd(II). IR (KBr, cm^{-1}): 3419(w), 3139(w), 2981(w), 2870(w), 1620(s), 1422(s), 1371(m), 1278(m), 1216(m), 1171(s), 1133(w), 1096(s), 1033(m), 1012(s), 849(s), 748(m), 675(m), 646(m); Elemental Anal. Calcd for $C_{13}H_{11}CdClO_3N_5$ (%): C, 36.02; H, 2.77; N, 16.16; Found (%): C, 35.94; H, 2.82; N, 16.21.

2.4. *Synthesis of $[Cd(Htmb)_2(Cl)_2(H_2O)_2]\cdot 4H_2O$ (2)*

Compound **2** was synthesized by the reaction of $Cd(Ac)_2\cdot 2H_2O$ (0.1 mmol, 26.6 mg), KCl (0.1 mmol, 7.5 mg), Htmb (0.1 mmol, 19.9 mg), methanol (8 mL), and water (2 mL) being mixed in a sealed Teflon-lined stainless steel vessel (25 mL) at 160°C for 5 days. After cooling to room temperature, colorless, block-like crystals were collected by filtration. Yield: 56% based on Cd(II). IR (KBr, cm^{-1}): 3423(w), 3136(w), 2984(w), 2873(w), 1627(s), 1552(s), 1438(s), 1214(m), 1172(s), 1133(w), 1094(s), 1036(m), 1021(s), 857(s), 759(m), 684(m), 648(m); Elemental Anal. Calcd for $C_{20}H_{28}CdN_{10}O_6Cl_2$ (%): C, 35.52; H, 3.55; N, 20.72; Found (%): C, 35.57; H, 3.64; N, 21.16.

2.5. *Synthesis of $[Cd(Htmb)_2(I)_2]$ (3)*

Compound **3** was synthesized by the reaction of $Cd(Ac)_2\cdot 2H_2O$ (0.1 mmol, 26.6 mg), KI (0.1 mmol, 16.6 mg), Htmb (0.1 mmol, 19.9 mg), and water (10 mL) being mixed in a sealed Teflon-lined stainless steel vessel (25 mL) at 100°C for 5 days. After cooling to room temperature, pale-yellow, block-like crystals were collected by filtration. Yield: 32% based on Cd(II). IR (KBr, cm^{-1}): 3418(w), 2897(w), 1623(s), 1547(s), 1464(s), 1276(m), 1216(m), 1170(s), 1133(w), 1089(s), 1036(m), 1017(s), 851(s), 748(m), 685(m), 645(m); Elemental Anal. Calcd for $C_{20}H_{16}CdN_{10}I_2$ (%): C, 31.47; H, 2.10; N, 18.36; Found (%): C, 31.62; H, 2.21; N, 18.54.

2.6. *Crystallographic data collection and structure determination*

Intensity data for Htmb and **1**–**3** were collected at 293 K on a Rigaku Saturn 724 CCD diffractometer equipped with graphite-monochromated Mo-Kα radiation ($\lambda = 0.71073$ Å). All structures were solved by direct methods and expanded using Fourier techniques. The non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms were assigned with common isotropic displacement factors and included in the final refinement using geometrical constraints. The final cycle of full-matrix least-squares refinement was based on observed reflections and variable parameters. All calculations were performed using the SHELXL-97 crystallographic software package [15]. Table 1 shows crystallographic data of Htmb and **1**–**3**. Selected bond distances and angles for Htmb and **1**–**3** are listed in table 2.

Table 1. Crystallographic data for Htmb and **1**–**3**.

Compound	Htmb	**1**	**2**	**3**
Empirical formula	$C_{10}H_9N_5$	$C_{13}H_{11}CdClO_3N_5$	$C_{20}H_{28}CdN_{10}O_6Cl_2$	$C_{20}H_{16}CdN_{10}I_2$
Formula weight	199.21	433.12	687.73	762.63
Crystal system	Orthorhombic	Triclinic	Monoclinic	Monoclinic
Space group	*Pbca*	$P\bar{1}$	*P2/c*	$P2_1/n$
Unit cell dimensions (Å, °)				
a	6.4648(13)	8.2991(17)	8.3548(17)	12.219(2)
b	9.841(2)	9.5661(19)	10.231(2)	14.345(3)
c	30.508(6)	11.528(2)	17.982(4)	15.274(3)
α	90.00	110.03(3)	90.00	90.00
β	90.00	96.53(3)	98.73(3)	104.14(3)
γ	90.00	105.21(3)	90.00	90.00
Volume (Å^3), Z	1941.0(7), 8	808.6(3), 2	1519.3(5), 2	2596.2(9), 4
Calculated density (g cm^{-3})	1.357	1.779	1.477	1.951
Absorption coefficient (mm^{-1})	0.090	1.536	0.943	3.247
$F(000)$	824.0	426.0	672.0	1440
Goodness-of-fit on F^2	1.312	0.905	1.023	1.189
Final R indices $[I > 2\sigma(I)]$	$R_1 = 0.0756$, $wR_2 = 0.1985$	$R_1 = 0.0364$, $wR_2 = 0.0928$	$R_1 = 0.0519$, $wR_2 = 0.1426$	$R_1 = 0.0520$, $wR_2 = 0.1426$
R indices (all data)	$R_1 = 0.0766$, $wR_2 = 0.1992$	$R_1 = 0.0429$, $wR_2 = 0.0998$	$R_1 = 0.0628$, $wR_2 = 0.1536$	$R_1 = 0.0572$, $wR_2 = 0.1472$
Largest difference peak and hole (e Å^{-3})	0.54 and −0.48	0.81 and −0.72	0.85 and −0.79	0.92 and −0.55

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

3. Results and discussion

3.1. *Luminescence properties*

The luminescence spectra of Htmb and **1**–**3** are determined in the solid state at room temperature. As can be seen from figure 1, Htmb displays an emission band at 384 nm upon photoexcitation at 290 nm, which can be attributed to the intraligand π–π^* transition. Compound **1** exhibits intense emission peaks at 381 nm when excited at 287 nm. Compound **2** exhibits intense emission peaks at 380 nm when excited at 291 nm. We note that the fluorescent intensity of **2** is weaker than that of **1**, probably due to quenching of water [16, 17]. Compared with Htmb, **3** exhibits a very weak emission band centered at 389 nm (ex = 291 nm). It can be presumed that the significantly weakened intensity of the emission band for **3** is attributed to competitive quenching of iodide [18, 19].

3.2. *Crystal structure*

The crystal structure of Htmb is shown in figure 2. The ligand crystallizes in the orthorhombic system, space group *Pbca*.

Single-crystal X-ray diffraction reveals that **1** crystallizes in the triclinic system, space group $P\bar{1}$, and the asymmetric unit consists of one Cd(II), one Htmb, one acetate, and one chloride. Cd(II) is six-coordinate, surrounded by two nitrogen atoms provided by two Htmb ligands (N1 and N4), two chloride atoms (Cl1, Cl2), and two oxygen atoms from one acetate forming a distorted octahedral environment, as depicted in figure 3. The bridging chlorides connect two Cd(II) cations, resulting in a Cd_2Cl_2 binuclear unit.

Table 2. Selected bond lengths (Å) and angles (°) for Htmb and **1**–**3**.

Htmb			
N4–C4	1.359(3)	N4–C5	1.381(4)
N5–C4	1.312(3)	N5–C10	1.394(4)
N1–C2	1.320(4)	N1–N2	1.342(3)
N1–C3	1.457(4)	C10–C5	1.392(4)
N3–C2	1.305(5)	N2–C1	1.271(4)
C1–N3	1.329(5)		
C4–N4–C5	106.4(2)	C4–N5–C10	104.7(2)
C2–N1–N2	107.3(3)	C2–N1–C3	130.2(3)
N2–N1–C3	122.3(3)	C5–C10–N5	109.5(2)
N5–C10–C9	130.0(3)	N5–C4–N4	113.5(2)
N5–C4–C3	124.6(2)	N4–C4–C3	121.9(2)
N1–C3–C4	111.2(2)	N4–C5–C10	105.8(2)
N4–C5–C6	132.3(3)	C1–N2–N1	106.8(3)
N2–C1–N3	111.1(3)	C1–N3–C2	105.9(3)
N3–C2–N1	109.0(4)		
1			
Cd1–N9	2.283(10)	Cd1–O1	2.329(10)
Cd1–N6	2.402(10)	Cd1–O2	2.477(10)
Cd1–Cl1	2.602(3)	Cd1–Cl2	2.653(3)
Cd2–N4	2.202(9)	Cd2–O3	2.239(9)
Cd2–N2A	2.448(11)	Cd2–O4	2.522(8)
Cd2–Cl2	2.607(3)	Cd2–Cl1	2.664(3)
N9–Cd1–O1	151.5(3)	N9A–Cd1–N6	89.3(3)
O1A–Cd1–N6	82.0(4)	N9–Cd1–O2	99.4(4)
O1–Cd1–O2	53.9(3)	N6A–Cd1–O2	90.5(3)
N9–Cd1–Cl1	109.9(3)	O1–Cd1–Cl1	96.6(3)
N6A–Cd1–Cl1	86.2(3)	O2–Cd1–Cl1	150.4(2)
N9–Cd1–Cl2	98.8(2)	O1–Cd1–Cl2	94.4(3)
N6A–Cd1–Cl2	168.3(2)	O2–Cd1–Cl2	96.4(3)
Cl1–Cd1–Cl2	83.18(9)	N4–Cd2–O3	151.9(3)
N4A–Cd2–N2	88.1(4)	O3A–Cd2–N2	83.6(4)
N4–Cd2–O4	99.1(3)	O3–Cd2–O4	54.5(3)
N2A–Cd2–O4	91.2(4)	N4–Cd2–Cl2	110.8(3)
O3–Cd2–Cl2	95.9(2)	N2A–Cd2–Cl2	88.9(3)
O4–Cd2–Cl2	150.1(2)	N4–Cd2–Cl1	97.2(3)
O3–Cd2–Cl1	94.6(3)	N2A–Cd2–Cl1	171.4(3)
O4–Cd2–Cl1	94.6(3)	Cl2–Cd2–Cl1	82.88(9)
2			
Cd1–N1	2.293(3)	Cd1–O2	2.364(4)
Cd1–O1	2.375(5)	Cd1–Cl1	2.6488(13)
Cd1–Cl1A	2.6488(13)	Cd1–N1A	2.293(3)
N1–Cd1–N1A	162.58(15)	N1–Cd1–O2	81.29(8)
N1A–Cd1–O2	81.29(8)	N1–Cd1–O1	98.71(8)
N1A–Cd1–O1	98.71(8)	O2–Cd1–O1	180.0
N1–Cd1–Cl1	88.18(8)	N1A–Cd1–Cl1	94.07(8)
O2–Cd1–Cl1	97.46(3)	O1–Cd1–Cl1	82.54(3)
N1A–Cd1–Cl1	94.07(8)	N1A–Cd1–Cl1A	88.18(8)
O2–Cd1–Cl1A	97.46(3)	O1–Cd1–Cl1A	82.54(3)
Cl1–Cd1–Cl1A	165.08(5)		
3			
Cd1–N5	2.254(4)	Cd1–N6	2.272(4)
Cd1–I1	2.7110(10)	Cd1–I2	2.7274(9)
N5–Cd1–N6	98.79(16)	N5–Cd1–I1	113.83(11)
N6–Cd1–I1	112.93(10)	N5–Cd1–I2	112.36(11)
N6–Cd1–I2	103.32(10)	I1–Cd1–I2	114.10(3)

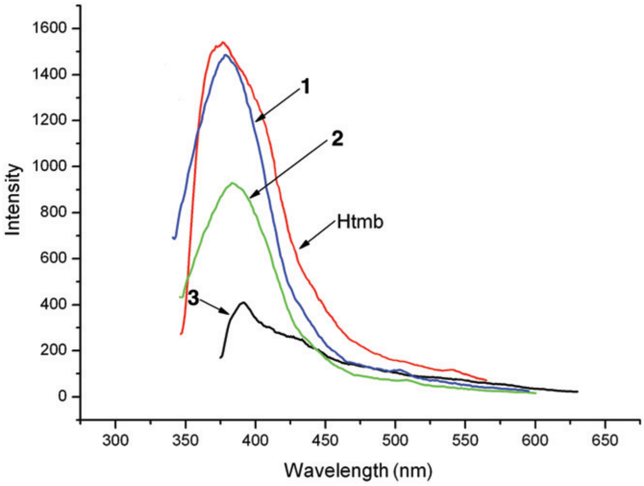

Figure 1. Solid-state photoluminescence of **1**–**3**.

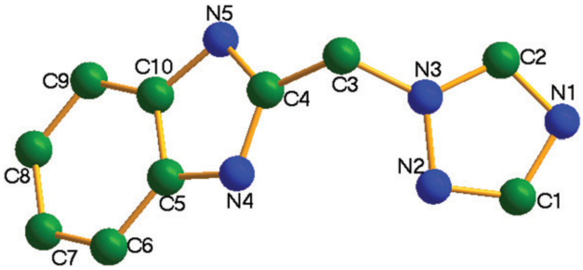

Figure 2. The molecular structure of Htmb with atom numbering. Hydrogen atoms have been omitted for clarity.

Htmb involves bidentate bridging coordination that joins binuclear units of $[Cd_2(Htmb)_4(Cl)_2(CH_3O_2)_2]$ and leads to a 1-D double chain (figure 4). Hydrogen bonds are present among CH_3OH, acetate, and benzoimidazole (N5···O5 $[x, y, z+1] = 2.756$ Å, O5···O2 $[x-1, y, z-1] = 2.810$ Å) that further link adjacent chains into a 2-D layer in the *ac* plane (figure S1). Adjacent layers are linked by π–π interactions between benzoimidazole rings with centroid–centroid distance of 3.68 Å to give a 3-D supramolecular structure (figure S2).

In contrast $[Cd(Hbimt)Cl_2(H_2O)]_n$ (Hbimt = 2-((benzoimidazol-yl)methyl)-1H-tetrazole), in which each Cd is six-coordinate by one oxygen of water, two nitrogen atoms from two different Hbimt ligands, and three chlorides forms a slight distorted octahedron. Hbimt adopts a bidentate bridging coordination that joins subunits of $[Cd_2(Hbimt)_4(Cl)_2(H_2O)_2]$ to form a 1-D stair-like chain [20]. Hence, structural differences between two Cd polymers can be attributed to the different coordination environment around Cd(II).

Compound **2** crystallizes in the monoclinic system, space group *P2*/*c*, and the asymmetric unit consists of one Cd(II), two Htmb, two chlorides, and two water molecules.

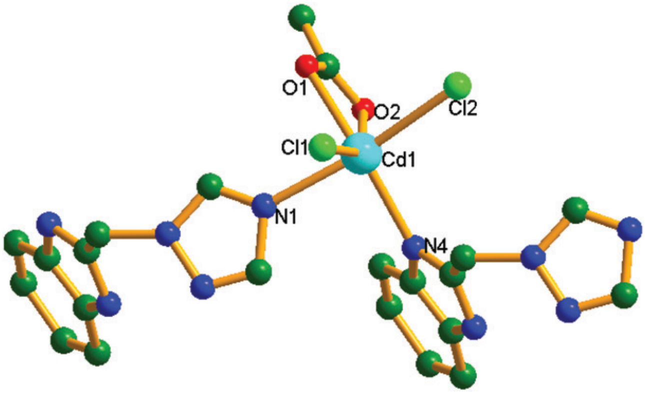

Figure 3. Coordination environment of Cd1 in **1**.

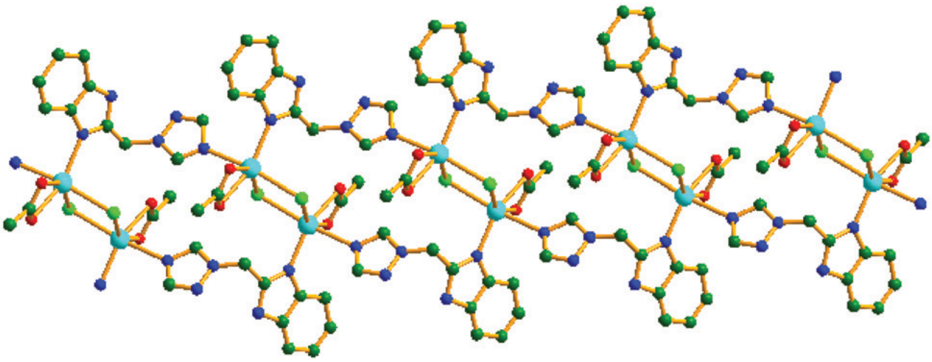

Figure 4. 1-D chain in **1**.

Each Cd is six-coordinate, surrounded by two nitrogen atoms provided by two Htmb (N1, N1A), two water molecules (O1, O2), and two chlorides (Cl1, Cl1A) to form a octahedral environment (figure 5). The bond lengths of Cd–O range from 2.364(4) to 2.375(5) Å and the bond lengths of Cd–N and Cd–Cl are 2.293(3) and 2.6488(13) Å, respectively. Bond angles of N1–Cd1–N1A, O1–Cd1–O2, and Cl1–Cd1–Cl1A are 162.58(15)°, 180.0°, and 165.08(5)°, respectively. Compared to **1**, reaction temperature plays a crucial role in tuning the coordination mode of Htmb. In **2**, the coordination environment around Cd is different than **1**, with Htmb monodentate (triazole group) to coordinate cadmium cations resulting in a mononuclear structure. Hydrogen bonds between coordinated water molecules and uncoordinated water molecules lead to an interesting water chain (figure 6a). The chains are further linked into a 2-D layer by chlorides (figure 6b). The $[Cd(Htmb)_2(Cl)_2(H_2O)_2]$ units join into a 3-D supramolecular network with the help of hydrogen interactions (figure S3).

Compared with **1** and **2**, introduction of iodides not only influences the coordinate mode of Htmb but also changes the coordination number of **3**. Compound **3** crystallizes in the monoclinic system, space group $P2_1/n$, and the asymmetric unit consists of one Cd(II), two Htmb, and two iodides. Each Cd is four-coordinate, surrounded by two

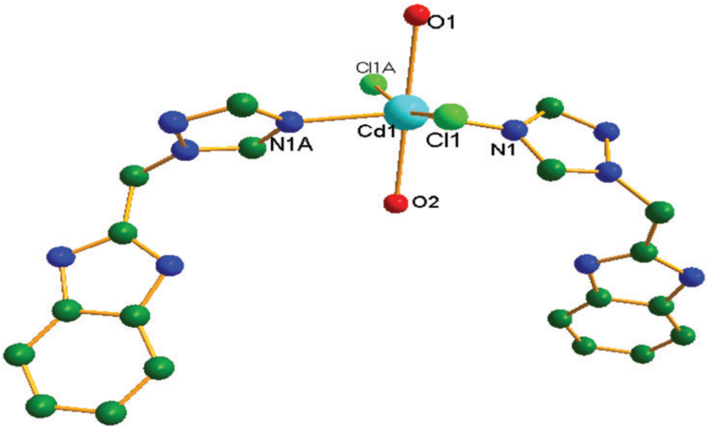

Figure 5. Coordination environment of Cd1 in **2**.

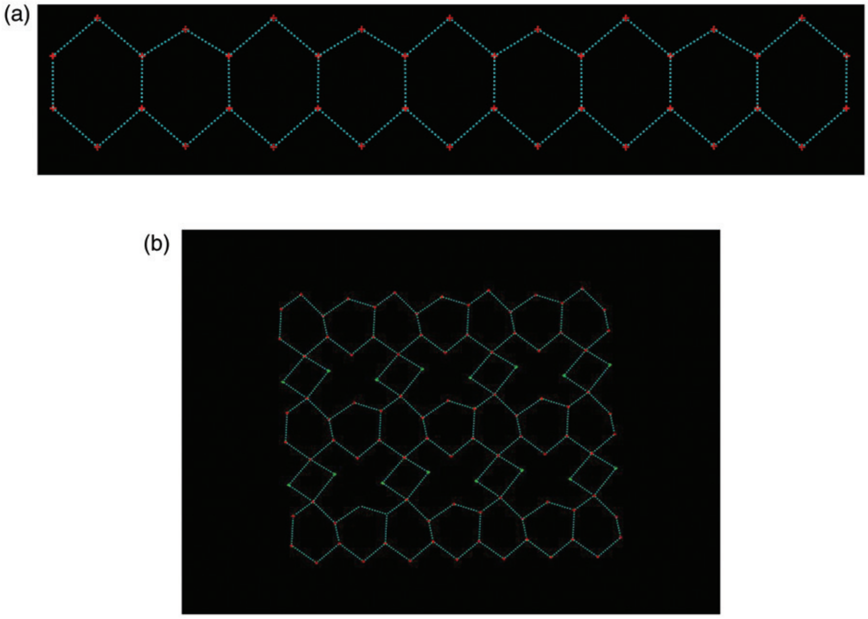

Figure 6. (a) The 1-D water chain in **2**; (b) the 2-D hydrogen system incorporating the chlorides in **2**.

nitrogen atoms provided by two Htmb (N1, N1A) and two iodides (I1, I2) to form a tetrahedral environment (figure 7). The bond lengths of Cd–I range from 2.7110(10) to 2.7274(9) Å and the bond lengths of Cd–N are 2.254(4)–2.272(4) Å. Bond angles of I1–Cd1–I2 and N5–Cd1–N6 are 114.10(3)° and 98.79(16)°, respectively. In **3**, Htmb employs monodentate coordination (benzoimidazole group) to coordinate cadmium bringing about a mononuclear structure. Hydrogen bonds formed between triazole and benzimidazole rings link [Cd(Htmb)$_2$(I)$_2$] units into 1-D zigzag chains (figure S4).

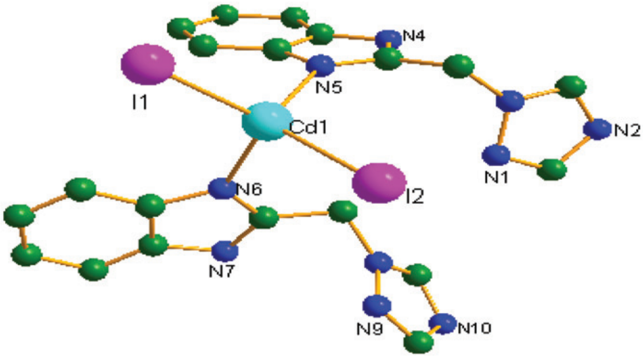

Figure 7. Coordination environment of Cd1 in **3**.

In addition, π–π interactions between benzimidazole rings and between triazole rings with centroid–centroid distance of 3.72 Å and 3.68 Å, respectively, give a 3-D supramolecular structure (figure S5).

4. Conclusion

Three new Cd(II) compounds have been synthesized by self-assembly of 2-(1H-triazol-1-ylmethyl)-1H-benzoimidazole (Htmb), Cd(II), and inorganic anions. In **1**–**3**, the Htmb adopts different coordinate modes to link Cd centers and forms hydrogen bonds that results in three 3-D supramolecular architectures. In addition, fluorescence in solid state have been observed for **1** and **2**, suggesting that the solids could be considered as potential luminescent materials.

Supplementary material

Crystallographic data for the structural analyses have been deposited to the Cambridge Crystallographic Data Center, CCDC Nos. 843262, 843263, 843264, and 843265. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (Fax: +44-1223-336033; Email: deposit@ccdc.cam.ac.uk, or http://www.ccdc.cam.ac.uk).

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