A New Cd(II) Coordination Compound Based on 4-(1,2,4-Triazol-4-yl)phenylacetic Acid: Synthesis, Structure and Photoluminescence Property Postprint

Authors: Mei-An Zhu, GUO Xing-Zhe, XIAO Li, CHEN Shui-Sheng

Date: 2017-11-05T00:00:00+00:00

Abstract

A new complex [Cd2(L)2(Cl)2(H2O)]n (1) was synthesized by reacting CdCl2 · 2.5H2O with 4-(1,2,4-triazol-4-yl)phenylacetic acid (HL) ligand. The structure of the complex was characterized by single-crystal X-ray diffraction, IR spectroscopy, elemental analysis and PXRD. Complex 1 crystallizes in triclinic, space group P21/c with a = 11.4303(8), b = 14.1792(10), c = 14.6857(10) Å, = 96.3780(10)º, V = 2365.4(3) Å3, Z = 4, C20H16Cl2N6O5Cd2, Mr = 716.09, Dc = 2.011 g/cm3, = 2.069-1, S = 1.051, F(000) = 1392, the final R = 0.0458 and wR = 0.0949 for 5402 observed reflections (I > 2 (I)). Complex 1 is a two-dimensional (2D) layer structure and non-covalent bonding interactions such as C-H··· and ··· extend the 2D to form a three-dimensional supramolecular polymer.

Full Text

A New Cd(II) Coordination Compound Based on 4-(1,2,4-Triazol-4-yl)phenylacetic Acid: Synthesis, Structure and Photoluminescence Property

ZHU Mei-An, GUO Xing-Zhe, XIAO Li, CHEN Shui-Sheng
College of Chemistry & Chemical Engineering, Fuyang Normal University, Fuyang 236041, China

ABSTRACT

A new complex, [Cd (L) (Cl) (H O)] (1), based on 4-(1,2,4-triazol-4-yl)phenylacetic acid (HL) containing triazolyl and carboxyl difunctional groups has been hydrothermally synthesized and characterized by single-crystal

X-ray diffraction, IR spectroscopy, elemental analysis, and PXRD. Complex 1 crystallizes in the monoclinic space group P2 /c with a = 11.4303(8), b = 14.1792(10), c = 14.6857(10) Å,   = 96.3780(10)°, V = 2365.4(3) $Å^3$, Z = 4, C H Cl N O Cd , M = 716.09, Dc = 2.011 g/cm^3,   = 2.069 mm^{1}, S = 1.051, F(000) = 1392, with final R = 0.0458 and wR = 0.0949 for 5402 observed reflections (I > 2 (I)). Complex 1 features a two-dimensional (2D) layer structure, and non-covalent bonding interactions such as C–H ⋯ and ⋯ stacking extend the 2D layers to form a three-dimensional supramolecular polymer.

Keywords: synthesis; supramolecular polymer; photoluminescent property
DOI: 10.14102/j.cnki.0254-5861.2011-1756

1. INTRODUCTION

The rational design and fabrication of metal-organic frameworks (MOFs) have flourished as an emerging research area due to their promising applications in guest molecule inclusion, gas and vapor storage, chemical sensing, magnetism, heterogeneous catalysis, and other fields [1-5]. Although synthetic conditions—including reaction temperature, solvent, pH of the medium, ligand-to-metal ratios, and choice of metal precursors—greatly influence the structures of the resulting complexes, the most critical factor for constructing desired MOFs is the judicious selection of appropriate linkers [6,7]. In addition, typical non-covalent interactions such as hydrogen bonding and / stacking (C—H ⋯) also play important roles in the assembly of supramolecular polymers [8-10].

Regarding ligand linkers, N- and/or O-donors have been extensively employed to build novel MOFs with interesting structures and properties [11,12]. Among N-donors, imidazole, triazole, and tetrazole analogues are widely used in MOF construction. Our groups have engaged in the design of 4-imidazole N-donor ligands, such as 1,4-di(1H-imidazol-4-yl)benzene and 1,3,5-tri(1H-imidazol-4-yl)benzene, which exhibit diverse coordination modes [13-15]. Furthermore, we have constructed diverse frameworks with favorable gas adsorption or selective gas adsorption properties based on metal-imidazolate units. Similarly, the O-donors of carboxylate groups display versatile coordination modes as well, suggesting that designable ligands incorporating multi-N and carboxylate groups may represent a useful strategy for constructing novel MOFs [16,17].

Therefore, our groups have further designed difunctional organic linkers combining carboxyl and 4-imidazolyl donors, such as 4-(1H-imidazol-4-yl)benzoic acid, which have proven to be good candidates for MOF construction in our previous studies [18]. Taking into account the favorable coordination ability of multi-N and O-donors, we synthesized the ligand 4-(1,2,4-triazol-4-yl)phenylacetic acid (HL) containing both triazolyl and carboxyl groups, which may exhibit rich coordination modes in MOF assembly. Herein, we report the synthesis and crystal structure of a new coordination polymer, [Cd (L) (Cl) (H O)] (1), obtained by reacting HL with CdCl ·2.5H O as an extension of our previous work.

---

2. EXPERIMENTAL

2.1 Materials and Measurements

All commercially available chemicals and solvents were of reagent grade and used as received without further purification. Elemental analyses were performed on a Perkin-Elmer 240C Elemental Analyzer. IR spectra were recorded on a Bruker Vector 22 FT-IR spectrophotometer using KBr pellets. Thermogravimetric analyses (TGA) were performed on a simultaneous SDT 2960 thermal analyzer under nitrogen at a heating rate of 10 °C/min. Powder X-ray diffraction (PXRD) patterns were measured on a Shimadzu XRD-6000 X-ray diffractometer with CuK (= 1.5418 Å) radiation at room temperature.

2.2 Synthesis of Complex [Cd (L) (Cl) (H O)] (1)

A mixture of HL (0.020 g, 0.1 mmol), CdCl ·2.5H O (0.022 g, 0.1 mmol), and 10 mL H O was adjusted to pH = 7 with 0.5 mol L ^{1} NaOH solution. The mixture was then sealed in a 20 mL Teflon-lined stainless-steel container and heated at 160 °C for 48 h. Colorless block crystals of 1 were collected by filtration with a yield of 42% and washed several times with water and ethanol. Anal. Calcd. (%) for C H Cl N O Cd : C, 33.54; H, 2.25; N, 11.74. Found (%): C, 33.33; H, 2.41; N, 11.61. IR (KBr): 3215 (w), 1591 (s), 1575 (vs), 1543 (m), 1529 (vs), 1395 (vs), 1243 (m), 1093 (s), 1037 (m), 1019 (m), 821 (m), 777 (s), 670 (w), 638 (w), 588 (w), 515 (w) cm ^{1}.

2.3 Crystal Structure Determination

Colorless crystals of complex 1 were selected for diffraction data collection at 296(2) K on a Bruker Smart Apex II CCD diffractometer equipped with graphite-monochromated Mo-K radiation (= 0.71073 Å). A total of 14109 reflections were collected for 1, of which 5402 (R = 0.0574) were independent in the range of 1.79 27.62° using a - scan mode. The structure was solved by direct methods with the SHELXS-97 program [19] and refined by full-matrix least-squares techniques on F^2 with SHELXL-97 [20]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions and refined using the riding model. The final refinement gave R = 0.0458, wR = 0.0949 (w = 1/[^{2}(F ^{2}) + (0.0572P)^2 + 0.4516P], where P = (F ^{2} + 2F_c^2)/3), R = 0.0574, (Δ/) = 0.000, S = 1.051, (Δ) = 1.230 and (Δ) = -1.193 e/Å^3 for 1. Selected bond distances and bond angles for complex 1 are listed in Tables 1 and 2, respectively.

---

3. RESULTS AND DISCUSSION

3.1 Crystal Structure of 1

Single-crystal X-ray diffraction analysis revealed that complex 1 crystallizes in the monoclinic system with space group P2 /c. The asymmetric unit of 1 contains two crystallographically independent Cd(II) atoms, two Cl anions, two L ligands, and one coordinated water molecule. As shown in Fig. 1 [Figure 1: see original paper], the Cd(1) atom exhibits octahedral coordination geometry with an N O Cl binding set, coordinated by two nitrogen atoms (N(1), N(4)) from two L ligands, two oxygen atoms (O(1D), O(4B)) from two other L ligands, one oxygen atom (O(7)) from a coordinated water molecule, and one Cl anion. Meanwhile, Cd(2) also displays octahedral coordination geometry with an NO Cl coordination sphere. The Cd–O distances range from 2.229(5) to 2.420(4) Å, while the Cd–N distances are 2.316(5)–2.382(5) Å, and the coordination angles around Cd(II) range from 73.27(6)° to 180.0° (Table 1).

A notable feature of the structure of 1 is that the HL ligands exhibit two distinct coordination modes coexisting within the same compound (Fig. 2 [Figure 2: see original paper]): (i) one acts as a -bridging linker, using one N atom to bridge one Cd(II) atom and two oxygen atoms from the carboxyl group in a -^{1}:^{1}-bridging mode to ligate two Cd(II) atoms; (ii) the other adopts a -bridging mode, using two N atoms to bridge two Cd(II) atoms and the carboxyl group in a -^{2}:^{1}-bridging mode to chelate two Cd(II) atoms. Two adjacent Cd(II) ions are alternately linked by one triazolate group, one carboxylate group, and one bridging Cl ion with distances of 3.994(7) and 4.056(7) Å to form a one-dimensional (1D) chain (Fig. 3 [Figure 3: see original paper]).

It is noteworthy that both types of L ligands connect Cd(II) atoms to form 1D chains, and these two distinct 1D chains intersect each other, creating a 1D helix chain structure (Fig. 4a [Figure 4: see original paper]). Similarly, there are two different Cl anions: one acts as a terminal coordination atom to balance the positive charges, while the other functions as a -bridging ligand to connect Cd(II) atoms. Through the bridging interactions of triazole and carboxylate groups together with Cl , the 1D chains are further connected into a two-dimensional (2D) layer structure (Fig. 4b [Figure 4: see original paper]).

Hydrogen bonding interactions exist within the 2D structure (C(1)···Cl(2) 3.56 Å, C(1)–H(1)···Cl(2) 148°; C(5)···N(5)a 3.48 Å, C(5)–H(5)···N(5) 160°; O(2)···O(7) 3.36 Å, O(2)–H(5)···O(7) 156°; C(8)···Cl(2) 3.55 Å, C(8)–H(8)···Cl(2) 165°) (Table 2), which further reinforce the stability of the complex. In the overall framework of 1, the 2D layers repeat in an ···AAA··· stacking sequence along the b axis, and numerous intramolecular - and C–H··· interactions exist among the aromatic rings, as shown in Fig. 5 [Figure 5: see original paper]. The benzene rings of the L ligands between adjacent 2D layers are parallel and separated by a centroid-centroid distance of 3.68 Å and a C–H··· distance of 2.96 Å [21,22]. These non-classical weak - and C–H··· interactions further link the 2D layers into a three-dimensional

(3D) supramolecular polymer (Fig. 5 [Figure 5: see original paper]).

3.2 IR Spectrum, Thermal Stability, and Powder X-ray Diffraction of 1

The infrared spectrum of the complex was recorded between 4000 and 450 cm ^{1}, with important assignments provided in the experimental section (Fig. 6 [Figure 6: see original paper]). Strong characteristic bands of the carboxylate group appear in the range of 1590–1529 cm ^{1} for asymmetric vibrations. The carboxylic acid of HL is deprotonated to form the L ligand, and the strong absorption band around 1590 cm ^{1} is attributed to the asymmetric stretching vibration of the C=O group, which is significantly lower than that of the protonated carboxylate group monomer (1695 cm ^{1}), indicating delocalization of the C=O double bond [23].

Complex 1 was subjected to thermogravimetric analysis (TGA) to assess the stability of the supramolecular architecture, with results shown in Fig. 7 [Figure 7: see original paper]. A total weight loss of 2.36% was observed for 1 around 90 °C, attributed to the loss of the coordinated water molecule (calcd. 2.51%). The residue remains stable up to approximately 380 °C. Powder XRD experiments were carried out to confirm the phase purity of the bulk sample (Fig. 8 [Figure 8: see original paper]), and the experimental pattern of the as-synthesized sample matches the corresponding simulated pattern, indicating phase purity.

3.3 Photoluminescent Property

Coordination polymers with d^{1} closed-shell metal centers and rationally selected conjugated organic spacers may exhibit excellent fluorescence properties, making them promising candidates for photoactive materials [24,25]. We investigated the solid-state fluorescence properties of complex 1 and the free HL ligand at room temperature. The free HL ligand shows an intense emission band at 440 nm upon excitation at 365 nm, which may be attributed to *→ transitions of the intraligand [26,27]. In contrast, complex 1 exhibits light blue emission with a maximum at 433 nm upon excitation at 355 nm (Fig. 9 [Figure 9: see original paper]). Compared with the free ligand, the emission band of complex 1 is blue-shifted by 7 nm. Such broad emission bands may be tentatively assigned to ligand-to-metal charge transfer (LMCT) [28,29]. Additionally, Fig. 9 shows that the luminescence intensity of 1 has increased relative to the free ligand under the same conditions, which likely originates from coordination interactions between the Cd(II) metal center and the ligand, thereby enhancing conformational rigidity and decreasing non-radiative energy loss [30]. Therefore, complex 1 shows potential as a hybrid inorganic-organic photoactive material.

REFERENCES

(1) Zhao, T.; Heering, C.; Boldog, I.; Domasevitch, K. V.; Janiak, C. A view on systematic truncation of tetrahedral ligands for coordination polymers. *CrystEngComm.* 2017, 19, 776–780.

(2) Ahmad, N.; Younus, H. A.; Chughtaia, A. H.; Verpoort, F. Metal-organic molecular cages: applications of biochemical implications. *Chem. Soc. Rev.* 2015, 44, 9–25.

(3) Yuan, S.; Qin, J. S.; Zou, L.; Chen, Y. P.; Wang, X.; Zhang, Q.; Zhou, H. C. Thermodynamically guided synthesis of mixed-linker Zr-MOFs with enhanced tenability. *J. Am. Chem. Soc.* 2016, 138, 6636—6642.

(4) Xiao, J.; Oktawiec, J.; Milner, P. J.; Long, J. R. Pore environment effects on catalytic cyclohexane oxidation in expanded Fe (dobdc) analogues Dianne. *J. Am. Chem. Soc.* 2016, 138, 14371—14379.

(5) Xiao, L.; Li, W. D.; Fang, X.; Jiang, L. Y.; Chen, S. S. Two three-dimensional supramolecular polymer built from mixed N-donor and carboxylate ligands. *Chin. J. Struct. Chem.* 2016, 35, 781–788.

(6) Zhang, W. Q.; Zhang, W. Y.; Wang, R. D.; Ren, C. Y.; Li, Q. Q.; Fan, Y. P.; Liu, B.; Liu, P.; Wang, Y. Y. Effect of coordinated solvent molecules on metal coordination sphere and solvent-induced transformations. *Cryst. Growth Des.* 2017, 17, 517–526.

(7) Yao, P. F.; Liu, H. F.; Huang, F. P.; Feng, F. L.; Qin, X. H.; Huang, M. L.; Yu, Q.; Bian, H. D. A family of Zn(II)/Cd(II) halide systems incorporating 5,5 -di(pyridin-2-yl)-3,3 -bi(1,2,4-triazole). *CrystEngComm.* 2016, 18, 938–947.

(8) Qiao, R.; Chen, S. S.; Sheng, L. Q.; Yang, S.; Li, W. D. Syntheses, crystal structures, and properties of four complexes based on polycarboxylate and imidazole ligands. *J. Solid State Chem.* 2015, 228, 199–207.

(9) Zhu, M. A.; Guo, X. Z.; Chen, S. S. Synthesis, crystal structure and luminescent property of a Zn(II) complex based on 4-imidazole-carboxylate ligand. *Chin. J. Struct. Chem.* 2017, 36, 1348 1354.

(10) Li, W. D.; Fang, X.; Qiao, R.; Chen, S. S. Non-covalent bonded 3D supramolecular architectures based on acid-base adducts. *Chin. J. Struct. Chem.* 2016, 35, 46–54.

(11) Zhang, Z. Y.; Xiao, L.; Chen, S. S.; Qiao, R.; Yang, S. A novel Zn(II) complex with 4-connected umc topology: synthesis, crystal structure and luminescent property. *Chin. J. Struct. Chem.* 2017, 36, 819 824.

(12) Wang, D.; Sun, L.; Hao, C.; Yan, Y.; Liang, Z. Lanthanide metal-organic frameworks based on a 1,2,3-triazole-containing tricarboxylic acid ligand

for luminescence sensing of metal ions and nitroaromatic compounds. *RSC Adv.* 2016, 6, 57828–57834.

(13) Chen, S. S.; Chen, M.; Takamizawa, S.; Chen, M. S.; Su, Z.; Sun, W. Y. Temperature dependent selective gas sorption of the microporous metal-imidazolate framework [Cu(L)] (H L = 1,4-di(1H-imidazol-4-yl)benzene). *Chem. Commun.* 2011, 47, 752–754.

(14) Chen, S. S.; Qiao, R.; Sheng, L. Q.; Zhao, Y.; Yang, S.; Chen, M. M.; Liu, Z. D.; Wang, D. H. Cadmium(II) and zinc(II) complexes with rigid 1-(1H-imidazol-4-yl)-3-(4H-tetrazol-5-yl)benzene and varied carboxylate ligands. *CrystEngComm.* 2013, 15, 5713–5725.

(15) Chen, S. S.; Wang, P.; Takamizawa, S.; Okamura, T. A.; Chen, M.; Sun, W. Y. Zinc(II) and cadmium(II) metal-organic frameworks with 4-imidazole containing tripodal ligand: sorption and anion exchange properties. *Dalton Trans.* 2014, 43, 6012–6020.

(16) Shao, Y. L.; Cui, Y. H.; Gu, J. Z.; Wu, J.; Wang, Y. W.; Kirillov, A. M. Exploring biphenyl-2,4,4 -tricarboxylic acid as a flexible building block for the hydrothermal self-assembly of diverse metal–organic and supramolecular networks. *CrystEngComm.* 2016, 18, 765–778.

(17) Pachfule, P.; Garai, B.; Banerjee, R. Functionalization and isoreticulation in a series of metal-organic frameworks derived from pyridinecarboxylates. *Inorg. Chem.* 2016, 55, 7200—7205.

(18) Chen, S. S.; Liu, Q.; Zhao, Y.; Qiao, R.; Sheng, L. Q.; Liu, Z. D.; Yang, S.; Song, C. F. New metal-organic frameworks constructed from the 4-imidazole-carboxylate ligand: structural diversities, luminescence, and gas adsorption properties. *Cryst. Growth Des.* 2014, 14, 3727—3741.

(19) Sheldrick, G. M. *SHELXS-97, Program for the Solution of Crystal Structure.* University of Göttingen, 1997.

(20) Sheldrick, G. M. *SHELXL-97, Program for the Refinement of Crystal Structure.* University of Göttingen, 1997.

(21) Ye, R. P.; Zhang, X.; Zhai, J. Q.; Qin, Y. Y.; Zhang, L.; Yao, Y. G.; Zhang, J. N-donor ligands enhancing luminescence properties of seven Zn/Cd(II) MOFs based on a large rigid -conjugated carboxylate ligand. *CrystEngComm.* 2015, 17, 9155–9166.

(22) Surov, A. O.; Solanko, K. A.; Bond, A. D.; Brandl, A. B.; Perlovich, G. L. Cocrystals of the antiandrogenic drug bicalutamide: screening, crystal structures, formation thermodynamics and lattice energies. *CrystEngComm.* 2016, 18, 4818–4829.

(23) Nakamoto, K. *Infrared and Raman Spectra of Inorganic and Coordinated Compounds*, 5th ed.; Wiley & Sons: New York, 1997.

(24) Wang, D. Z.; Fan, J. Z.; Jia, D.; Du, C. C. Zinc and cadmium complexes based on bis-(1H-tetrazol-5-ylmethyl/ylethyl)-amine ligands: structures and photoluminescence properties. *CrystEngComm.* 2016, 18, 6708-6723.

(25) Xing, K.; Fan, R.; Gao, S.; Wang, X.; Du, X.; Wang, P.; Fang, R.; Yang, Y. Controllable synthesis of Zn/Cd(II) coordination polymers: dual-emissive luminescent properties, and tailoring emission tendency under varying excitation energies. *Dalton Trans.* 2016, 45, 4863-4878.

(26) Sun, Y. X.; Sun, W. Y. Zinc(II)- and cadmium(II)-organic frameworks with 1-imidazole-containing and 1-imidazolecarboxylate ligands. *CrystEngComm.* 2015, 17, 4045-4063.

(27) Singh, D.; Nagaraja, C. M. Auxiliary ligand-assisted structural variation of Cd(II) metal-organic frameworks showing 2D → 3D polycatenation and interpenetration: synthesis, structure, luminescence properties, and selective sensing of trinitrophenol. *Cryst. Growth Des.* 2015, 15, 3356—3365.

(28) Yang, L. B.; Wang, H. C.; Fang, X. D.; Chen, S. J.; Xu, Q. Q.; Zhu, A. X.; Yang, Z. A series of Zn(II) and Cd(II) coordination compounds based on 4-(4H-1,2,4-triazol-4-yl)benzoic acid: synthesis, structure and photoluminescence properties. *CrystEngComm.* 2016, 18, 130-142.

(29) Xue, Z.; Sheng, T.; Wang, Y.; Hu, S.; Wen, Y.; Wang, Y.; Li, H.; Fu, R.; Wu, X. A series of d^1 coordination polymers constructed with a rigid tripodal imidazole ligand and varied polycarboxylates: syntheses, structures and luminescence properties. *CrystEngComm.* 2015, 17, 2004-2012.

(30) Xu, J.; Bai, Z. S.; Chen, M. S.; Su, Z.; Chen, S. S.; Sun, W. Y. Metal-organic frameworks with six- and four-fold interpenetration and their photoluminescence and adsorption property. *CrystEngComm.* 2009, 11, 2728-2733.

Table 1. Selected Bond Lengths (Å) and Bond Angles (°) of [Cd (L) (Cl) (H O)]

Dist.		Dist.	
Cd(1)-N(4)	2.315(5)	Cd(1)-O(4)#B	2.228(5)
Cd(1)-O(7)	2.329(4)	Cd(1)-O(1)#D	2.340(4)
Cd(1)-N(1)	2.361(5)	Cd(1)-Cl(1)	2.5292(18)
Cd(2)-O(3)#B	2.344(4)	Cd(2)-N(2)#C	2.381(5)
Cd(2)-O(2)#A	2.401(4)	Cd(2)-O(1)#A	2.421(4)
Cd(2)-Cl(2)	2.4788(17)	Cd(2)-Cl(1)	2.4896(18)

Angle		Angle	
O(4)#B-Cd(1)-N(4)	92.3(2)	O(4)#B-Cd(1)-O(7)	170.44(18)

Angle		Angle	
N(4)-Cd(1)-O(7)	82.15(19)	O(4)#B-Cd(1)-O(1)#D	89.63(17)
N(4)-Cd(1)-O(1)#D	82.43(17)	O(7)-Cd(1)-O(1)#D	81.96(15)
O(4)#B-Cd(1)-N(1)	97.66(19)	N(4)-Cd(1)-N(1)	157.11(18)
O(7)-Cd(1)-N(1)	84.94(17)	O(1)#D-Cd(1)-N(1)	77.10(15)
O(4)#B-Cd(1)-Cl(1)	100.90(14)	N(4)-Cd(1)-Cl(1)	100.15(15)
O(7)-Cd(1)-Cl(1)	87.78(12)	O(1)#D-Cd(1)-Cl(1)	169.00(11)
N(1)-Cd(1)-Cl(1)	98.14(13)	O(3)#B-Cd(2)-N(2)#C	79.85(18)
O(3)#B-Cd(2)-O(2)#A	168.89(16)	N(2)#C-Cd(2)-O(2)#A	93.13(17)
O(3)#B-Cd(2)-O(1)#A	116.08(16)	N(2)#C-Cd(2)-O(1)#A	76.03(15)
O(2)#A-Cd(2)-O(1)#A	53.39(14)	O(3)#B-Cd(2)-Cl(2)	88.72(12)
N(2)#C-Cd(2)-Cl(2)	151.19(13)	O(2)#A-Cd(2)-Cl(2)	93.56(12)
O(1)#A-Cd(2)-Cl(2)	85.70(10)	O(3)#B-Cd(2)-Cl(1)	96.06(12)
N(2)#C-Cd(2)-Cl(1)	91.61(13)	O(2)#A-Cd(2)-Cl(1)	92.70(11)
O(1)#A-Cd(2)-Cl(1)	142.16(11)	Cl(2)-Cd(2)-Cl(1)	116.00(7)

Symmetry transformations: A: -1-x, -0.5+y, 1.5-z; B: 1-x, -0.5+y, 1.5-z; C: -x, -0.5+y, 1.5-z; D: 1+x, y, z

---

Table 2. Hydrogen Bonding Interactions for Complex 1 (Å, °)

D-H ⋯ A	H ⋯ A	D ⋯ A	D-H ⋯ A
C(1)-H(1) ⋯ Cl(2)	-	3.560(8)	148°
C(5)-H(5) ⋯ N(5)a	-	3.478(9)	160°
C(8)-H(8) ⋯ Cl(2)	-	3.550(7)	165°

Symmetry code: (a) -x, 0.5+y, 1.5-z

Fig. 1. Coordination environment of Cd(II) in complex 1 with ellipsoids drawn at 30% probability level. Hydrogen atoms were omitted for clarity (Symmetry codes: (A) -1-x, -0.5+y, 1.5-z; (B) 1-x, −0.5+y, 1.5−z; (C) -x, −0.5+y, 1.5−z; (D) 1+x, y, z)

Fig. 2. Coordination modes of L ligands in complex 1

Fig. 3. Cl and carboxylate-bridged 1D Cd(II) chains in 1

Fig. 4. (a) 1D helix chain and (b) 2D network structure of 1

Fig. 5. 3D supramolecular structure constructed from 2D layers stacked in an AAA sequence along the b axis, linked by ⋯ and C-H ⋯ interactions

Fig. 6. IR spectrum of complex 1

Fig. 7. TGA curve of complex 1

Fig. 8. Simulated and experimental XRPD patterns of complex 1

Fig. 9. Solid-state photoluminescent spectra of HL and complex 1 at room temperature

Note: Figure translations are in progress. See original paper for figures.

Source: ChinaXiv —Machine translation. Verify with original.