

# Halogen Bonding in the Assembly of a 1D Cadmium(II) Polymer Based on Chlorendic Acid (HET)

Pei-Pei Cui,<sup>[b]</sup> Lun-Feng Cui,<sup>[c]</sup> Liang-Liang Zhang,<sup>[a]</sup> and Dao-Feng Sun\*<sup>[a,b]</sup>

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**Abstract.** A new complex based on chlorendic acid (HET),  $[\text{Cd}_8(\text{HET})_8(\text{DMF})_4(\text{H}_2\text{O})_{12}] \cdot 8\text{DMF}$  (**1**) was synthesized by liquid evaporate method from the mixture of HET and  $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ . Single crystal X-ray analysis reveals that the structure of complex **1** features a one-dimensional (1D) wave chain that is further assembled into

three-dimensional (3D) framework directed by supramolecular interactions, including hydrogen bond,  $\text{Cl} \cdots \text{Cl}$  halogen bond, and so on. To the best of our knowledge, this is the first metal-organic coordination polymer based on chlorendic acid (HET). The luminescent property and thermal stability of complex **1** were also discussed.

## Introduction

With the development of supramolecular chemistry and crystal engineering, the rational design and synthesis of metal-organic coordination polymers has attracted much attention, not only for their intriguing variety of architectures and topologies but also owing to their potential applications in catalysis, gas absorption, ion exchange, luminescent, and so on.<sup>[1–7]</sup> Among them, many works have focused on low-dimensional metal-organic frameworks (MOFs), such as 1D ladders, 1D helical chains, 1D zigzag chains, 1D metal-organic tubes, 1D double or triple stranded chains with their omnifarious conformations.<sup>[8–13]</sup> Remarkably, for many ligands including halogen atoms the halogen bonding has been discussed.<sup>[14,15]</sup> The reason is that the halogen bonding exhibits characteristics comparable to the hydrogen bonding with regard to directionality and strength.<sup>[16,17]</sup> The coexistence of halogen-related interactions in combination with metal coordination within a given crystalline compound, usually obtained accidentally, has been systematically summarized.<sup>[18]</sup> Attempted assembly of discrete coordination complexes using halogen bonding or halogen and halogen atoms interactions into one- or two-dimensional (1D or 2D) supramolecular structures has proven its difficulty. The effect of halogen-related interactions in the assembly of high-

dimensional coordination polymers remains largely unexplored and needs more elaborate and systematic studies.<sup>[19,20]</sup>

Recently, our group focuses on the design and synthesis of functional MOFs with special properties based on multitopic organic ligands. In this article, we select chlorendic acid (HET) as the assembly ligand. There are many reasons to be considered. On the one hand, chlorendic acid (HET) is an effective intermediate material for many chemical compounds, because of excellent flame retardant, corrosion prevention, and solidifies property.<sup>[21–23]</sup> As far as we know, no metal-organic coordination polymers based on this ligand were reported. On the other hand, HET contains a lot of chlorine atoms, which leads to the possibility of forming halogen bonding. Furthermore, halogen bonding is the noncovalent interaction, where halogen atoms function as electrophilic species, which is important in supramolecular chemistry.<sup>[24]</sup>

Herein, we report a new coordination polymer  $[\text{Cd}_8(\text{HET})_8(\text{DMF})_4(\text{H}_2\text{O})_{12}] \cdot 8\text{DMF}$  (**1**) based on HET and cadmium ion, which featured a 1D wave chain and further assembled into a 3D supramolecular architecture stably by van der Waals force, such as hydrogen bond and  $\text{Cl} \cdots \text{Cl}$  halogen bond.

## Results and Discussion

### Crystal Structure of Compound **1**

Single-crystal X-ray diffraction analysis reveals that compound **1** crystallizes in monoclinic  $P2_1/c$  space group. The asymmetric unit contains two  $\text{Cd}^{\text{II}}$  ions, two HET ligands, three coordinated  $\text{H}_2\text{O}$  molecules as well as one coordinated and two uncoordinated dimethylformamide (DMF) molecules. The coordination environment of cadmium ions in **1** is shown in Figure 1. The  $\text{Cd}^{\text{II}}$  ion adopts a distorted octahedral arrangement, which is six-coordinate by four carboxylate oxygen atoms from two different HET molecules and two oxygen atoms from one coordinated  $\text{H}_2\text{O}$  molecule and one coordi-

\* Prof. Dr. D.-F. Sun  
E-Mail: dfsun@upc.edu.cn, dfsun@sdu.edu.cn

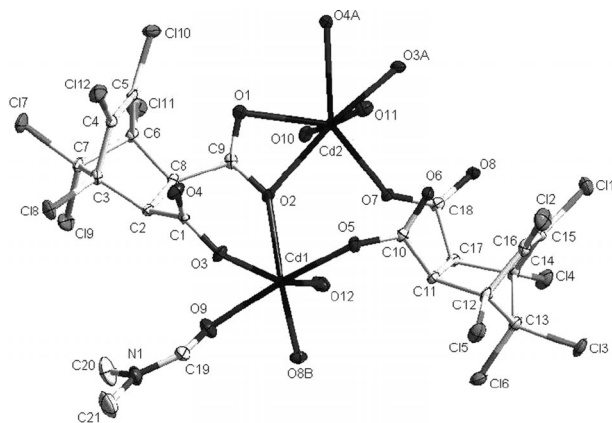
[a] College of Science  
China University of Petroleum (East China)  
Qingdao Shandong 266580, P. R. China

[b] Key Lab of Colloid and Interface Chemistry  
Ministry of Education, School of Chemistry and Chemical Engineering  
Shandong University  
Jinan, 250199, P. R. China

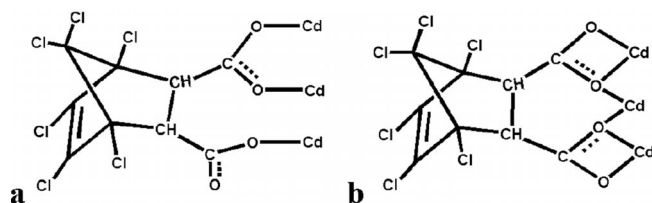
[c] Zhuli Middle School  
Hanting District  
Weifang, Shandong, 261111, China

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nated DMF molecule. However, the coordination environment of Cd2 is different from Cd1. Cd2 ion is coordinated by seven oxygen atoms, in which five oxygen atoms come from three HET ligands, whereas another two oxygen atoms come from coordinated water molecules. O1 and O2 come from one carboxylate group with a chelating mode, which is similar to O3 and O4. The Cd–O<sub>HET</sub> distances range from 2.266 (2) to 2.556 (3) Å, Cd–O<sub>w</sub> distances range from 2.249 (3) to 2.267 (3) Å and the Cd–O<sub>DMF</sub> distance is 2.310 (3) Å. The bond angles O–Cd–O are in the range from 53.55(8) to 173.47(10)°, which are comparable to those of reported Cd<sup>II</sup> coordination polymers.<sup>[25]</sup> The HET ligand exhibits two kinds of coordination modes as shown in Scheme 1: (a) in the *a*-type, one carboxylate group adopts bidentate bridging mode to link two cadmium ions, whereas the other one bridging another cadmium ion; (b) in the *b*-type HET ligand, each carboxylate group adopts chelating mode to link one cadmium ion, at the same time one oxygen atom of the carboxylate group bridges another cadmium ion.

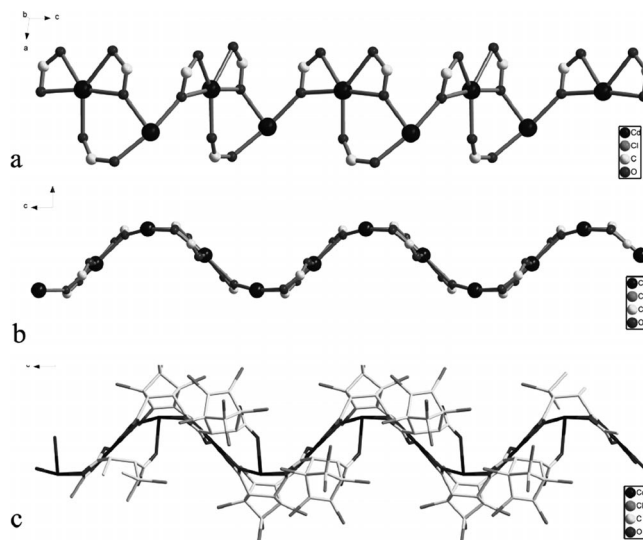


**Figure 1.** Coordination environment of compound **1**. Hydrogen atoms are omitted for clarity.



**Scheme 1.** Coordination modes of the ligand HET.

Thus, Cd1 and Cd2 ions were connected by *a*-type HET and *b*-type HET ligands along *a* axis to generate a 1D wave chain with Cd–O–C and Cd–O–Cd rods (Figure 2a). And the 1D wave chain looks like sine function image of mathematics (Figure 2b). Besides, the 1D Cd–O–C rods in complex **1** are slightly different from other reported results<sup>[25]</sup> and the nearest Cd–Cd distance in the wave chain is 3.956 Å.

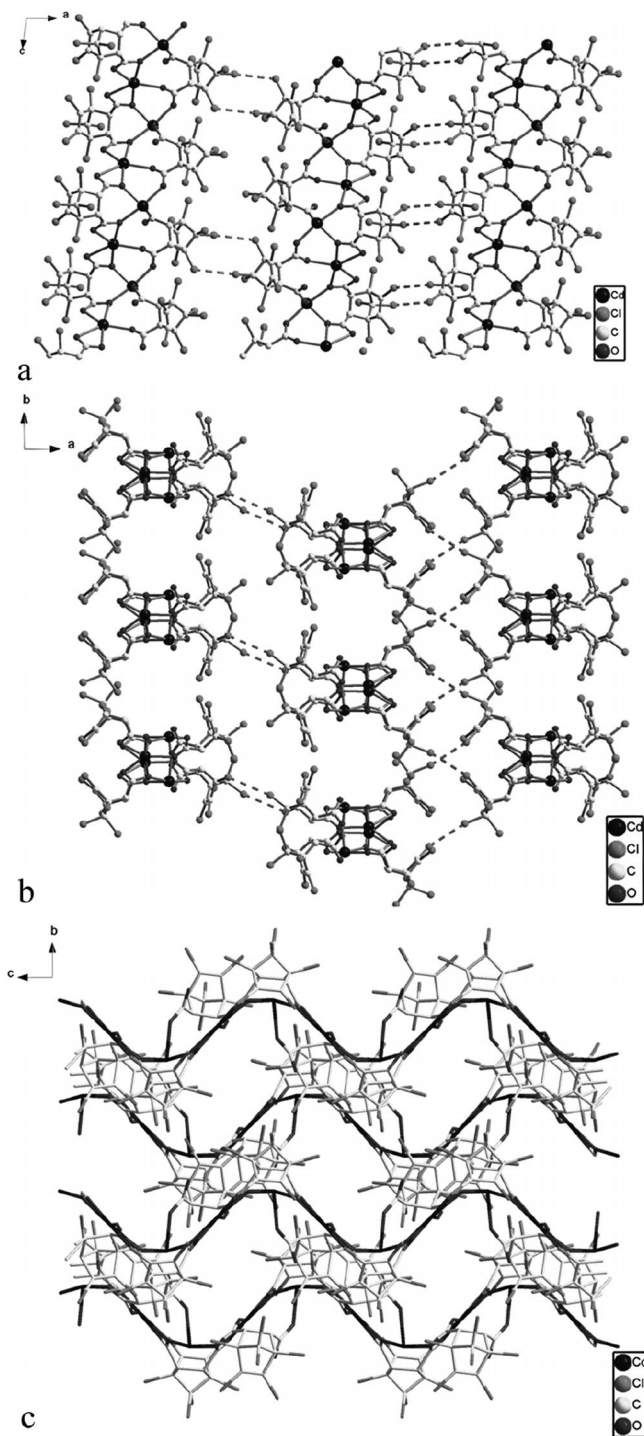


**Figure 2.** (a) The 1D rod-shaped SBU; (b) 1D wave chain existed in **1** (along *a* axis). Cl molecules are omitted; (c) View along *a* axis. Coordinated water and DMF molecules and hydrogen atoms are omitted for clarity.

Recently, many researchers discuss the role of supramolecular interactions in the assembly of coordination polymers. For example, *Politzer* and *Goebel* et al. discussed halogen bonds.<sup>[26]</sup> Herein, hydrogen and halogen bonds were also discussed, because the weak forces were suggested to act as familiar structure-direction tools in coordination polymers. In compound **1**, there exist hydrogen bonding interactions between the coordinated carboxyl oxygen atoms and coordinated water oxygen atoms, and between coordinated water oxygen atoms and oxygen atoms of the uncoordinated DMF molecules. The distances between the neighboring oxygen atoms in the molecule forming hydrogen bond are O10...O5 2.756 Å, O11...O14 2.729 Å, and O12...O13 2.756 Å. The detailed hydrogen-bonding parameters are listed in Table S2 (Supporting Information). Besides, weak Cl...O interactions (Cl5...O13 3.1374 Å) exist between the chlorine atoms and oxygen atoms of the uncoordinated DMF molecules in compound **1**. Interestingly, the distances between the nearest Cl7 atoms and Cl10 atoms (3.430 Å) (C5–Cl10–Cl7 152.1°, C7–Cl7–Cl10 167.9°) from different chains are shorter than the sum of the van der Waals radii of the two atoms (ca. 3.6 Å),<sup>[27]</sup> indicating Cl...Cl halogen bonding. Moreover, there exist van der Waals interaction between different 1D wave chains with the distance of Cl3...Cl4 3.617 Å. In brief, significant supramolecular interactions were also implicated for the reinforcement and overall stability of the crystal lattice. So the final structure of **1** turned to a 3D supramolecular framework (Figure 3).

### Thermal Stability and Photoluminescent Properties

Complex **1** is stable in air at room temperature. To examine the thermal stability, thermalgravimetric analysis (TGA) was carried out in a nitrogen atmosphere from room temperature to 600 °C (Figure S1, Supporting Information). The TGA study on an as-isolated crystalline sample of **1** shows a 11.8% weight

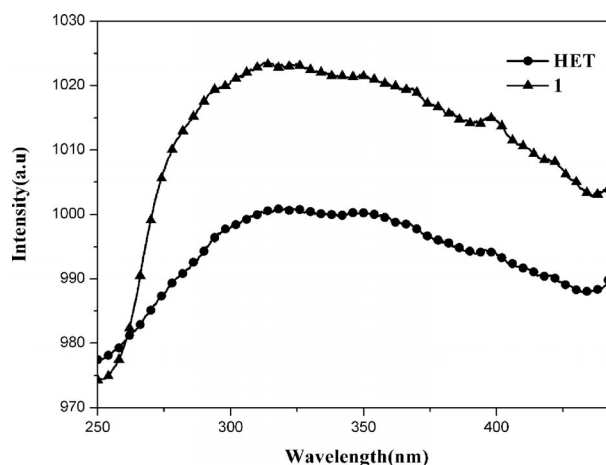


**Figure 3.** Supramolecular interactions in **1**: (a) Cl3...Cl4 and Cl7...Cl10 interactions are shown as dashed lines at the *b* axis. (b) 3D Supramolecular architecture of **1**: viewed along the *c* axis. (c) 3D Supramolecular architecture of **1**: viewed along the *a* axis. Coordinated water and DMF molecules and hydrogen atoms are omitted for clarity.

loss from 103.5 to 155.0 °C, corresponding to the loss of eight uncoordinated DMF molecules (calcd: 11.5%). The second gradual weight loss of 16.1% from 155.0 to 255.4 °C corresponds to the loss of twelve coordinated water molecules and

four coordinated DMF molecules (calcd: 10.0%). After 255.4 °C, the decomposition of complex **1** occurs.

Luminescent properties of  $d^{10}$  transition metal complexes have been well reported.<sup>[28]</sup> The organic ligands and their coordination modes have great effect on the emission wavelengths and luminescent mechanisms. In order to well understand the luminescent property, the absorption spectrum of complex **1** and free ligand (HET) were measured in solid state at room temperature. As shown in Figure 4, complex **1** and HET display luminescent emission bands at 313 nm and 320 nm upon 250 nm excitation. The emission of HET was ascribed to the  $\pi^* \rightarrow n$  or  $\pi^* \rightarrow \pi$  electronic transitions. Because the  $Cd^{II}$  ion is difficult to oxidize or to reduce due to its  $d^{10}$  electronic configuration, the emissions of the complex is neither metal-to-ligand charge transfer nor ligand-to-metal charge transfer. The emission of complex **1** can probably be assigned to the intraligand or ligand-to-ligand charge transition as a result of the resemblance of the emission spectra in comparison with those of the free ligand.<sup>[29]</sup>



**Figure 4.** Solid-state excitation spectra of complex **1** and HET at room temperature.

## Conclusions

[Cd<sub>8</sub>(HET)<sub>8</sub>(DMF)<sub>4</sub>(H<sub>2</sub>O)<sub>12</sub>]<sub>8</sub>DMF (**1**) was synthesized and characterized based on Cd<sup>II</sup> and chlorendic acid (HET). The interesting structural feature in **1** is that the 1D wave chain looks like sine function image of mathematics. Meanwhile, hydrogen and halogen bonds were found. The 1D coordination polymer of **1** is further stabilized to form 3D structure via interchain supra-molecular interactions. The solid-state luminescent property and thermal stability of complex **1** were also discussed.

## Experimental Section

**Materials and Instrumentation:** All reagents and solvents employed were commercially available and used without further purification. Elemental analyses (C and H) were determined with an elemental Vario EL III analyzer. Photoluminescence spectra were measured with a Hitachi F-7000 Fluorescence Spectrophotometer. Thermogravimetric

analyses were performed with a NETZSCH TG 209 F1 Iris® Thermogravimetric Analyser from room temperature to 600 °C at a heating rate 10 °C·min<sup>-1</sup> in a nitrogen atmosphere (20 mL·min<sup>-1</sup>). Powder X-ray diffraction (PXRD) data were collected with a Philips X'Pert Pro MPD X-ray diffractometer with Cu-K<sub>α</sub> radiation equipped with an X'Celerator detector.

**Synthesis of [Cd<sub>8</sub>(HET)<sub>8</sub>(DMF)<sub>4</sub>(H<sub>2</sub>O)<sub>12</sub>·8DMF (1):** The new complex was prepared by liquid evaporate method. In a 18 × 180 mm test tube, Cd(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O (0.05 mmol, 15 mg) was suspended in water (5 mL), while HET (5 mg, 0.013 mmol) was suspended in *N,N*-dimethylformamide (DMF, 5 mL). Afterwards they were mixed and the mixture was stirred for 30 min. The mixture was filtered and the filtrate was allowed to evaporate at room temperature for 3 weeks. The colorless block crystals (6 mg) were collected, washed with water and dried in the air. Yield: 56% (based on HET). Elemental analyses for C<sub>108</sub>H<sub>124</sub>Cd<sub>8</sub>Cl<sub>48</sub>N<sub>12</sub>O<sub>56</sub> (5086.99): calcd. C 25.50; N 3.30; H 2.46%; found: C 25.45; N 3.29; H 2.60%.

**X-ray Structure Analyses:** Single crystal of complex **1** with appropriate dimensions was chosen under an optical microscope and coated with high vacuum grease (Dow Corning Corporation) quickly before being mounted on a glass fiber for data collection. Data were collected at room temperature with a Bruker Apex II Image Plate single-crystal diffractometer with graphite-monochromated Mo-K<sub>α</sub> radiation source (λ = 0.71073 Å) operating at 50 kV and 30 mA in ω scan mode for **1**. A total of 44 × 5.00° oscillation images were collected, each being exposed for 5.0 min. Absorption correction was applied by correction of symmetry-equivalent reflections using the Multi-scan program. The highest possible space group was chosen. The structure was solved by direct methods using SHELXS-97<sup>[30]</sup> and refined on F<sup>2</sup> by full-matrix least-squares procedures with SHELXL-97.<sup>[31]</sup> Atoms were located from iterative examination of difference F-maps following least-squares refinements of the earlier models. Hydrogen atoms on organic ligands were placed in calculated positions and included as riding atoms with isotropic displacement parameters 1.2–1.5 times U<sub>eq</sub> of the attached carbon atoms. Hydrogen atoms attached to oxygen in **1** were located by difference Fourier maps and refined subject to the constraint O–H = 0.85 Å, and U<sub>iso</sub>(H) = 1.2U<sub>eq</sub>(O). The calculation of halogen bonding and the structure were examined using the Addsym subroutine PLATON to assure that no additional symmetry could be applied to the models. Crystal structure pictures were obtained using Diamond v3.1f and ChemDraw. For compound **1**, crystal data and collection and parameters are summarized in Table 1. Selected bond lengths and angles and the parameters of hydrogen bond are listed in Table S1 and Table S2.

**Supporting Information** (see footnote on the first page of this article): Selected bond lengths and angles, hydrogen bonding parameters, TG curve, experimental and simulated PXRD patterns for compound **1**.

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**Table 1.** Crystal data for compound **1**.

Empirical formula	C <sub>108</sub> H <sub>124</sub> Cd <sub>8</sub> Cl <sub>48</sub> N <sub>12</sub> O <sub>56</sub>
Formula weight	5086.99
Temperature /K	293
Crystal system	monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> /Å	30.5959(15)
<i>b</i> /Å	11.2878(5)
<i>c</i> /Å	12.8294(6)
<i>α</i> /°	90.00
<i>β</i> /°	97.2970(10)
<i>γ</i> /°	90.00
Volume /Å <sup>3</sup>	4394.9(4)
<i>Z</i>	1
ρ <sub>calcd.</sub> /mg·mm <sup>-3</sup>	1.922
μ /mm <sup>-1</sup>	1.760
<i>F</i> (000)	2504
2θ range for data collection	2.68 to 56.1°
Index ranges	−38 ≤ <i>h</i> ≤ 40 −11 ≤ <i>k</i> ≤ 14 −14 ≤ <i>l</i> ≤ 16
Reflections collected	10288
Independent reflections	8039[R(int) = 0.0357]
Data / restraints / parameters	10288 / 0 / 529
Goodness-of-fit on <i>F</i> <sup>2</sup>	0.955
Final <i>R</i> indexes [ <i>I</i> ≥ 2σ ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0351, <i>wR</i> <sub>2</sub> = 0.0817
Final <i>R</i> indexes [all data]	<i>R</i> <sub>1</sub> = 0.0542, <i>wR</i> <sub>2</sub> = 0.0984
Largest diff. peak/hole /e·Å <sup>-3</sup>	0.624 / −0.577

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