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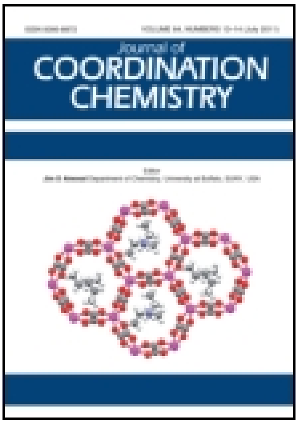

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Complexes based on ferrocenecarboxylate ligands: steric hindrance induced by ferrocenyl groups

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Three metal complexes with ferrocenecarboxylate ligands, $[M_2(\eta^2\text{-FcCOO})_2(\mu_2\text{-}\eta^2\text{-FcCONHCH}_2\text{COO})_2(\text{phen})_2]\cdot n\text{H}_2\text{O}$ [M = Pb, $n = 6$ (**1**) and M = Cd, $n = 2$ (**2**)] and $[\text{Cd}(\text{FcCONHCH}_2\text{COO})(\mu_2\text{-FcCONHCH}_2\text{COO})(2,2'\text{-bipy})(\text{H}_2\text{O})]_n$ (**3**) (FcCOOH = ferrocenemonocarboxylic acid, $\text{FcCONHCH}_2\text{COOH}$ = *N*-ferrocenylformylglycine, phen = 1,10-phenanthroline, 2,2′-biby = 2,2′-bipyridine), were synthesized and characterized by elemental analysis, IR, and single crystal X-ray diffraction analysis. Structural studies revealed that **1** and **2** have similar binuclear structures, but **3** exhibits a 1-D chain structure. The difference in the structures of ferrocenylcarboxylate-containing cadmium(II) complexes is due to steric hindrance of ferrocenyl groups.

Keywords: Ferrocenecarboxylate; Steric hindrance effect; Complex; Crystal structure

1. Introduction

Ferrocene-containing compounds have been applied as ligands for the preparation of metal complexes in coordination chemistry due to aromaticity, redox activities, stability, and low toxicity of the ferrocene moiety [1]. Introduction of ferrocene can bring unusual electrical properties [2], magnetism [3], catalysis [4], nonlinear optics (NLO) [5], and medical properties [6] for the corresponding metal complexes. Among ferrocene-containing ligands, ferrocenecarboxylates [7–9] are widely used because of the versatile coordination modes of carboxylate, such as chelate [10, 11], unidentate [12, 13], μ_2-bidentate [14–16], μ_2-η^2-, μ_3-tridentate [8, 17], and μ_3-η^2-tetradentate [9], providing the possibility of constructing complexes with structural diversity. Most reported metal ferrocenecarboxylate complexes are mononuclear [10, 12, 13, 18] and binuclear [14, 15] with simple structures, few are high-nuclearity complexes [16, 19] and polymers [8, 20]. This might be attributed to steric hindrance induced by ferrocenyl groups.

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However, the steric influence imposed by ferrocene on the construction of ferrocene-containing complexes has not yet been investigated systematically.

We present herein the syntheses and structures of two dinuclear complexes, $[M_2(\eta^2\text{-FcCOO})_2(\mu_2\text{-}\eta^2\text{-FcCONHCH}_2\text{COO})_2(\text{phen})_2] \cdot n\text{H}_2\text{O}$ [$M = \text{Pb}$, $n = 6$ (**1**) and $M = \text{Cd}$, $n = 2$ (**2**)], and a 1-D chain coordination polymer, $[\text{Cd}(\text{FcCONHCH}_2\text{COO})(\mu_2\text{-FcCONHCH}_2\text{COO})(2,2'\text{-bipy})(\text{H}_2\text{O})]_n$ (**3**), which involve two kinds of ferrocenecarboxylate ligands with different steric hindrance. The steric hindrance induced by ferrocenyl groups in the cadmium(II) complexes is discussed in detail.

2. Experimental

2.1. *Materials and methods*

All reagents and solvents were purchased commercially and used without purification. *N*-ferrocenylformylglycine was prepared according to a literature method [21]. IR spectra were recorded from 4000 to 400 cm^{-1} on a Perkin-Elmer PE Spectrum One FT/IR spectrometer. Elemental analyses were performed on a Perkin-Elmer PE 2400 II CHN elemental analyzer.

2.2. *Synthesis of the complexes*

2.2.1. Synthesis of $[\text{Pb}_2(\eta^2\text{-FcCOO})_2(\mu_2\text{-}\eta^2\text{-FcCONHCH}_2\text{COO})_2(\text{phen})_2] \cdot 6\text{H}_2\text{O}$ (1). An aqueous solution (5 mL) of $\text{Pb(OAc)}_2 \cdot 3\text{H}_2\text{O}$ (0.38 g, 1.0 mmol) was added to a methanol solution (10 mL) of *N*-ferrocenylformylglycine (0.29 g, 1.0 mmol) and NaOH (0.04 g, 1.0 mmol). Subsequently, a methanol solution (5 mL) of 1,10-phenanthroline monohydrate (0.20 g, 1.0 mmol) and a methanol solution (5 mL) of ferrocenemonocarboxylic acid (0.23 g, 1.0 mmol) with NaOH (0.04 g, 1.0 mmol) were added with stirring. The resulting solution was further stirred at ambient temperature for 12 h and then filtered. The filtrate was allowed to evaporate in the dark, giving orange-colored block crystals of **1** suitable for single crystal X-ray diffraction analysis after 15 days (Yield: 50%, based on Pb). Anal. Calcd for $\text{C}_{72}\text{H}_{70}\text{Pb}_2\text{Fe}_4\text{N}_6\text{O}_{16}$ (1913.12) (%): C, 45.20; H, 3.69; N, 4.39. Found (%): C, 45.42; H, 3.84; N, 4.16. IR data (KBr pellets, cm^{-1}): 3435(s), 1620(m), 1559(m), 1514(m), 1387(m), 1355(w), 1279(m), 1104(m), 849(w), 726(m).

2.2.2. Synthesis of $[\text{Cd}_2(\eta^2\text{-FcCOO})_2(\mu_2\text{-}\eta^2\text{-FcCONHCH}_2\text{COO})_2(\text{phen})_2] \cdot 2\text{H}_2\text{O}$ (2). Complex **2** was prepared in a method similar to that for **1** using $\text{Cd(OAc)}_2 \cdot 2\text{H}_2\text{O}$ (0.27 g, 1.0 mmol) instead of $\text{Pb(OAc)}_2 \cdot 3\text{H}_2\text{O}$. Orange-colored needle-like crystals were obtained by slow evaporation of the filtrate in the dark after 20 days (Yield: 47%, based on Cd). Anal. Calcd for $\text{C}_{72}\text{H}_{62}\text{Cd}_2\text{Fe}_4\text{N}_6\text{O}_{12}$ (1651.48) (%): C, 52.36; H, 3.78; N, 5.09. Found(%): C, 52.62; H, 3.91; N, 4.89. IR data (KBr pellets, cm^{-1}): 3430(s), 1637(m), 1591(w), 1549(s), 1536(s), 1390(m), 1358(w), 1282(m), 1104(m), 821(w), 728(m).

2.2.3. Synthesis of [Cd(FcCONHCH$_2$COO)(μ_2-FcCONHCH$_2$COO)(2,2′-bipy)(H$_2$O)]$_n$ (3). An aqueous solution (5 mL) of Cd(OAc)$_2 \cdot 2H_2O$ (0.13 g, 0.5 mmol) was added to a solution of *N*-ferrocenylformylglycine (0.29 g, 1.0 mmol) and NaOH (0.04 g, 1.0 mmol) in methanol (10 mL). Then a methanol solution (5 mL) of 2,2′-bipyridine (0.08 g, 0.5 mmol) was added dropwise. The resulting solution was further stirred for 12 h and then filtered. The filtrate was allowed to evaporate in the dark, giving orange-colored block crystals suitable for single crystal X-ray diffraction after 15 days (Yield: 45%, based on Cd). Anal. Calcd for $C_{36}H_{34}CdFe_2N_4O_7$ (858.77) (%): C, 50.06; H, 3.99; N, 6.52. Found (%): C, 50.29; H, 3.81; N, 6.75. IR data (KBr pellets, cm^{-1}): 3406(s), 3306(m), 1630(s), 1585(s), 1557(s), 1402(m), 1402(m), 1390(m), 1296(m), 1104(w), 773(m).

2.3. *X-ray crystallographic studies*

Suitable single crystals of **1**–**3** were selected and mounted in air onto thin glass fibers. X-ray diffraction data were collected on a Bruker SMART APEX CCD diffractometer at 293(2) K using Mo-Kα radiation ($\lambda = 0.71073$ Å) by multi-scan mode. The SAINT program was used for integration of the diffraction profiles. The structures were solved by direct methods using the SHELXS-97 program package and refined against F^2 by full-matrix least-squares with SHELXL-97 [22]. All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms on carbon were set in calculated positions and refined as riding. The crystallographic data are summarized in table 1 and selected bond lengths and angles are listed in table 2. Hydrogen bonds for **1**–**3** are listed in table 3.

3. Results and discussion

3.1. *Structural descriptions of 1 and 2*

Complexes **1** and **2**, both of which crystallize in the triclinic space group $P\bar{1}$, present similar centrosymmetric binuclear structures, as shown in figure 1. Thus, only the structure of **1** is discussed here in detail. The Pb(II) in **1** is seven coordinate in distorted monocapped trigonal prism geometry by two nitrogen atoms (N2, N3) from 1,10-phenanthroline, three carboxylate oxygen atoms (O2, O3, O3^a) from two *N*-ferrocenylformylglycine ligands, and two carboxylate oxygen atoms (O4, O5) from one ferrocenemonocarboxylate. The Pb–O2, Pb–O3^a, and Pb–O3 distances are 2.569(6), 2.718(6), and 2.803(6) Å, respectively, in the range of those reported in [23, 24]. The seven-coordinate lead is located on one side of the plane defined by N3, O2, O3, and O3^a leaving the other side for the stereochemically active lone pair, which reveals a hemidirected geometry for Pb(II) in **1** [24, 25]. However, the Cd(II) ion in **2** presents a holdirected monocapped trigonal prism geometry with the Cd–O and Cd–N bond lengths comparable to those in related compounds [26]. The carboxylates of FcCOO$^-$ in **1** chelate and the carboxylates of FcCONHCH$_2$COO$^-$ are μ_2-η^2-tridentate bridging. Two μ_2-η^2-bridging carboxylates from two FcCONHCH$_2$COO$^-$ ligands connect two Pb(II) ions to build a binuclear structure of **1**.

Table 1. Crystallographic data and refinement summary for **1**–**3**.

Complexes	**1**	**2**	**3**
Empirical formula	$C_{72}H_{70}Pb_2Fe_4N_6O_{16}$	$C_{72}H_{62}Cd_2Fe_4N_6O_{12}$	$C_{36}H_{34}CdFe_2N_4O_7$
Formula weight	1913.12	1651.48	858.77
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$
Unit cell dimensions (Å, °)			
a	11.597(11)	10.664(4)	19.2337(14)
b	13.098(13)	12.771(4)	20.1215(14)
c	13.171(12)	13.734(5)	8.9404(6)
α	108.755(15)	67.094(5)	90
β	91.749(16)	68.272(6)	98.4030(10)
γ	114.270(15)	88.832(6)	90
Volume (Å^3), Z	1696(3), 1	1583.7(9), 1	3422.9(4), 4
Calculated density (g cm^{-3})	1.873	1.732	1.666
Absorption coefficient (mm^{-1})	5.853	1.622	1.508
$F(000)$	940	832	1736
Reflections collected	8920	8154	18,247
Independent reflections	5955 ($R_{int} = 0.0392$)	5511 ($R_{int} = 0.0391$)	6033 ($R_{int} = 0.0323$)
Data/restraints/parameters	5955/0/451	5511/0/433	6033/0/451
Goodness-of-fit on F^2	1.012	0.966	1.069
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0477$, $wR_2 = 0.0851$	$R_1 = 0.0461$, $wR_2 = 0.0793$	$R_1 = 0.0270$, $wR_2 = 0.0664$
R indices (all data)	$R_1 = 0.0775$, $wR_2 = 0.0986$	$R_1 = 0.0950$, $wR_2 = 0.0958$	$R_1 = 0.0354$, $wR_2 = 0.0689$
Largest difference peak and hole (e Å^{-3})	0.940 and −1.599	0.744 and −0.583	0.468 and −0.364

There are six guest water molecules per formula unit of **1**. One kind of water molecule with oxygens labeled as O6 form hydrogen bonds O6–H6A $\cdots$ O1^b and O6–H6B $\cdots$ O5 with $O_{acylamide}$ of $FcCONHCH_2COO^-$ and $O_{carboxylate}$ of $FcCOO^-$ from adjacent binuclear units. Another kind of water molecule with oxygens labeled as O7 are hydrogen bonded to the $O_{carboxylate}$ of $FcCONHCH_2COO^-$ and the oxygens (O8^b) from guest water molecules, forming H-bonds O7–H7B $\cdots$ O2 and O7–H7A $\cdots$ O8^b, while the guest water molecules with oxygens labeled as O8 form H-bonds O8–H8A $\cdots$ O1 and O8–H8B $\cdots$ O6 with the $O_{acylamide}$ of $FcCONHCH_2COO^-$ and the guest water oxygens (O6). Adjacent dinuclear units of **1** are connected *via* these hydrogen bonds with O $\cdots$ O distances and O–H $\cdots$ O angles of 2.68–3.39 Å and 137–179°, respectively, forming a 1-D chain, as shown in figure 2.

Different from **1**, there exists only two guest water molecules per formula unit of **2**, also involved in hydrogen bonding, forming hydrogen bonds O6–H6A $\cdots$ O5^a and O6–H6B $\cdots$ O1^b with $O_{carboxylate}$ of $FcCOO^-$ and $O_{acylamide}$ of $FcCONHCH_2COO^-$ from adjacent binuclear units. The O $\cdots$ O distances and O–H $\cdots$ O angles are 2.825(6) Å and 151.5° for the former and 2.795(7) Å and 178.9° for the latter (table 3). With these H-bond interactions, **2** is extended into a 1-D chain, as shown in figure 3.

3.2. *Structural description of 3*

Single-crystal X-ray diffraction analysis reveals that **3** is a 1-D chain coordination polymer crystallizing in the monoclinic space group $P2_1/c$. Figure 4 shows the

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

1			
Pb1–O5	2.432(6)	O5–Pb1–N3	123.71(19)
Pb1–O4	2.548(6)	O4–Pb1–N3	83.14(19)
Pb1–N2	2.556(6)	N2–Pb1–N3	62.3(2)
Pb1–O2	2.569(6)	O2–Pb1–N3	126.90(18)
Pb1–N3	2.675(7)	O5–Pb1–O3^a	93.0(2)
Pb1–O3^a	2.718(6)	O4–Pb1–O3^a	73.05(18)
Pb1–O3	2.803(6)	N2–Pb1–O3^a	153.11(18)
O5–Pb1–O4	51.92(19)	O2–Pb1–O3^a	120.62(16)
O5–Pb1–N2	77.4(2)	N3–Pb1–O3^a	105.4(2)
O4–Pb1–N2	81.43(17)	O5–Pb1–O3	79.2(2)
O5–Pb1–O2	80.92(19)	O4–Pb1–O3	117.12(19)
O4–Pb1–O2	132.5(2)	N2–Pb1–O3	128.1(2)
N2–Pb1–O2	83.04(18)	O2–Pb1–O3	47.79(17)
2			
Cd1–O5	2.430(4)	O4–Cd1–O3	121.87(14)
Cd1–O4	2.354(4)	O2–Cd1–O3	54.47(14)
Cd1–N2	2.385(5)	N2–Cd1–O3	138.71(16)
Cd1–O2	2.360(4)	N3–Cd1–O5	145.67(16)
Cd1–N3	2.318(5)	O4–Cd1–O5	54.42(14)
Cd1–O3^a	2.508(4)	O2–Cd1–O5	101.53(15)
Cd1–O3	2.429(4)	N2–Cd1–O5	86.66(15)
N3–Cd1–O4	97.58(16)	O3–Cd1–O5	87.80(14)
N3–Cd1–O2	102.57(16)	N3–Cd1–O3^a	84.51(16)
O4–Cd1–O2	155.41(15)	O4–Cd1–O3^a	80.07(13)
N3–Cd1–N2	70.72(17)	O2–Cd1–O3^a	115.56(15)
O4–Cd1–N2	86.69(14)	N2–Cd1–O3^a	150.09(15)
O2–Cd1–N2	86.79(16)	O3–Cd1–O3^a	69.90(16)
N3–Cd1–O3	126.25(16)	O5–Cd1–O3^a	106.50(14)
3			
Cd1–O4	2.2307(17)	O5^a–Cd1–N2	80.35(8)
Cd1–O1	2.2633(17)	O4–Cd1–N1	83.28(7)
Cd1–O5^b	2.3288(18)	O1–Cd1–N1	148.75(7)
Cd1–N2	2.352(2)	O5^a–Cd1–N1	125.02(7)
Cd1–N1	2.363(2)	N2–Cd1–N1	68.55(7)
Cd1–O7	2.3863(18)	O4–Cd1–O7	94.66(6)
O4–Cd1–O1	124.68(7)	O1–Cd1–O7	83.27(6)
O4–Cd1–O5^b	86.24(7)	O5^a–Cd1–O7	154.28(7)
O1–Cd1–O5^b	75.28(6)	N2–Cd1–O7	116.25(7)
O4–Cd1–N2	132.43(7)	N1–Cd1–O7	80.50(7)
O1–Cd1–N2	95.59(7)		

Symmetry codes: for **1**: ^{a} $-x+1,\ -y+1,\ -z+1$; for **2**: ^{a} $-x+1,\ -y+1,\ -z+1$; for **3**: ^{b} $x,\ -y+1/2,\ z-1/2$.

coordination environment of Cd(II) in **3**. The Cd(II) is six coordinate in a distorted octahedral geometry by two nitrogen atoms (N1, N2) from 2,2′-bipyridine, three carboxylato oxygen atoms (O1, O4, O5^b) from three *N*-ferrocenylformylglycine ligands, and one oxygen atom (O7) from coordinated water molecule.

Complex **3** has two kinds of $FcCONHCH_2COO^-$ with different coordination of the carboxylate. One ligand is monodentate, whereas the other is μ_2-O,O′ bridging. The μ_2-O,O′ bridging $FcCONHCH_2COO^-$ connect adjacent Cd(II) ions into a 1-D chain with a shortest Cd$\cdots$Cd distance of 5.3789(4) Å. The two kinds of $FcCONHCH_2COO^-$ ligands are arranged regularly along the chain with all monodentate $FcCONHCH_2COO^-$ ligands on one side of the chain and all μ_2-O,O′

Table 3. Hydrogen bonds (Å and °) for **1**–**3**.

D–H···A	*d* (D–H)	*d* (H···A)	*d* (D···A)	∠DHA
1				
N1–H1···O4^{a}	0.86	2.15	3.001(9)	172.2
O6–H6A···O1^{b}	0.85	2.04	2.838(10)	155.6
O6–H6B···O5	0.85	1.97	2.818(9)	179.1
O7–H7A···O8^{b}	0.85	2.07	2.841(15)	151.9
O7–H7B···O2	0.85	2.13	2.820(9)	137.4
O8–H8A···O1	0.85	2.55	3.386(16)	168.5
O8–H8B···O6	0.85	1.89	2.687(13)	154.9
2				
N1–H1···O4^{a}	0.86	1.98	2.801(6)	160.4
O6–H6A···O5^{a}	0.85	2.05	2.825(6)	151.5
O6–H6B···O1^{b}	0.85	1.95	2.795(7)	178.9
3				
N3–H3A···O3^{a}	0.88	2.05	2.852(3)	151.5
N4–H4A···O6^{b}	0.87	2.04	2.895(3)	165.2
O7–H7A···O2	0.85	1.87	2.693(3)	165.2
O7–H7B···O1^{a}	0.85	2.19	2.971(2)	152.5
O7–H7B···O5	0.85	2.29	2.907(3)	129.8

Symmetry codes: for **1**: ^{a} $-x+1$, $-y+1$, $-z+1$; ^{b} $-x$, $-y+1$, $-z+1$; for **2**: ^{a} $-x+1$, $-y+1$, $-z+1$; ^{b} $x-1$, y, z; for **3**: ^{a} x, $-y+1/2$, $z+1/2$; ^{b} x, $-y+1/2$, $z-1/2$.

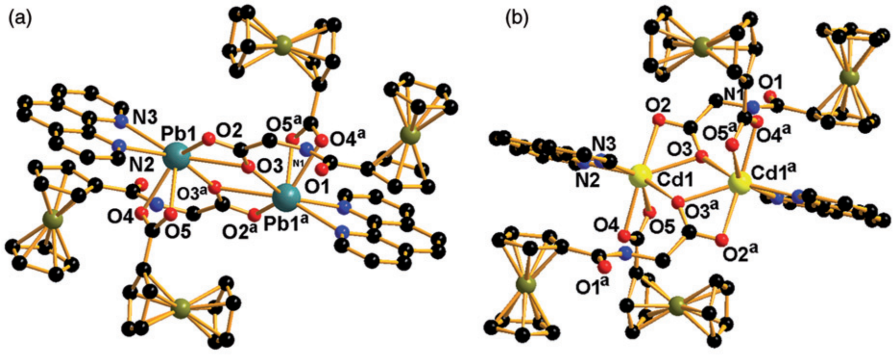

Figure 1. The perspective view of **1** (a) and **2** (b). Hydrogen atoms and guest water molecules are omitted for clarity. Symmetry codes: ^{a} $-x+1$, $-y+1$, $-z+1$.

bridging $FcCONHCH_2COO^-$ ligands on the other side, as shown in figure 5. There exist hydrogen bonds N–H···O between amino groups and carbonyl oxygens and O–H···O hydrogen bonds between coordinated water molecules and uncoordinated carboxylato oxygens, as shown in figure 5 and table 3. These hydrogen bonds further stabilize the 1-D chains. The pyridyl rings from adjacent 1-D chains overlap partly with a dihedral angle of 2.239° between the two adjacent pyridyl planes, a distance of 3.5787(1) Å from the center of one pyridyl ring to the adjacent pyridyl plane and an offset angle of 28.113°, indicating $\pi\cdots\pi$ stacking interactions between the adjacent pyridyl rings, forming a 2-D supramolecular sheet (figure 6) in the plane parallel to the *bc* plane.

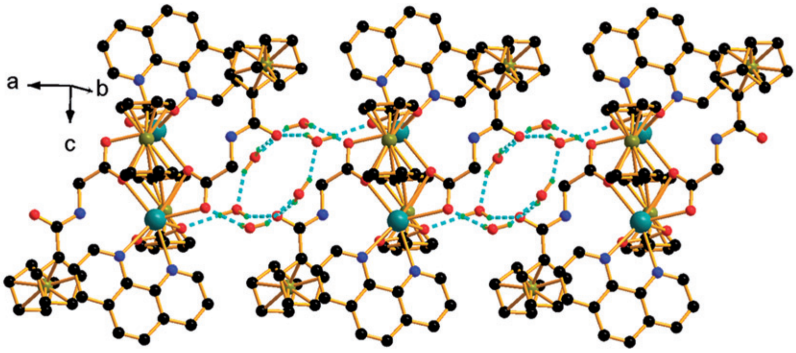

Figure 2. 1-D chain of **1** formed by intermolecular H-bonds (indicated by broken lines).

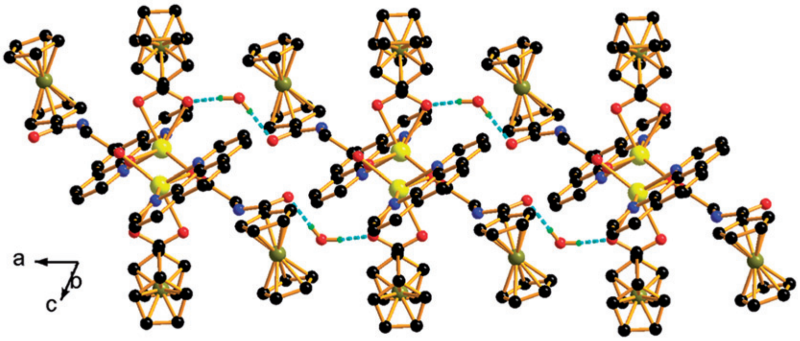

Figure 3. 1-D chain of **2** formed by intermolecular H-bonds (indicated by broken lines).

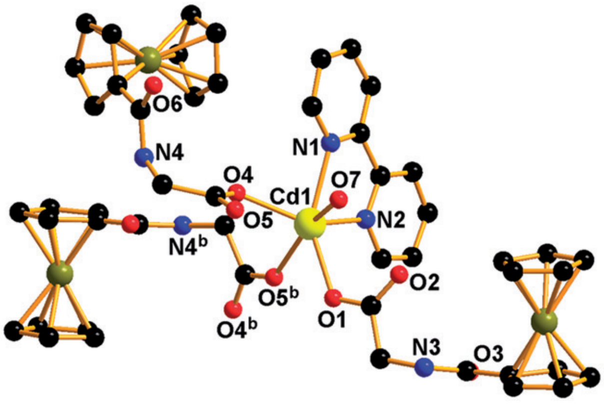

Figure 4. Molecular structure of **3** showing the coordination environment of Cd(II). Hydrogen atoms are omitted for clarity. Symmetry code: ^{b} $x, -y+1/2, z-1/2$.

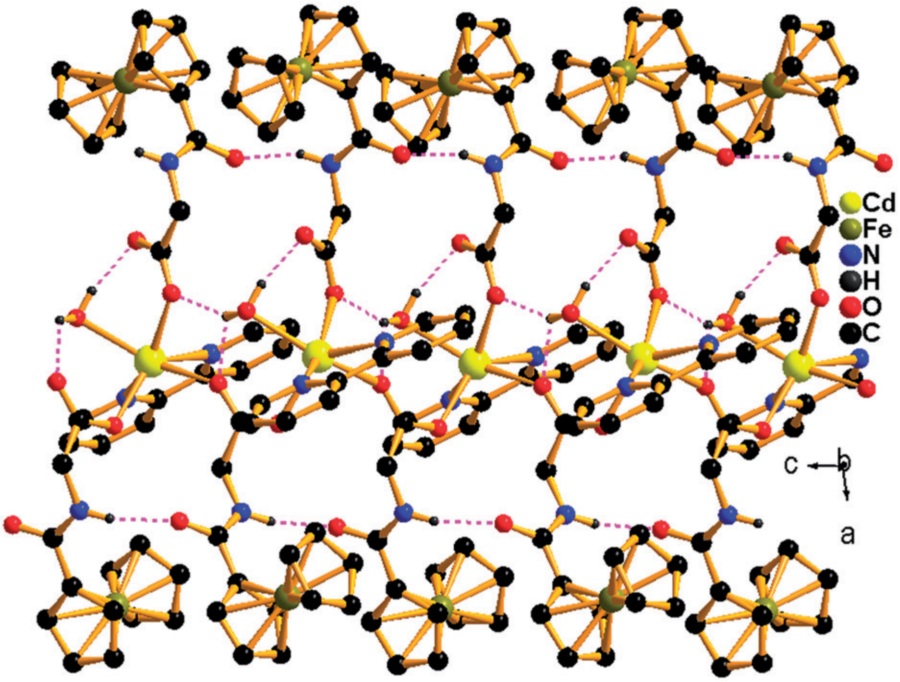

Figure 5. 1-D chain of **3**. Hydrogen atoms not involved in hydrogen bonds are omitted for clarity.

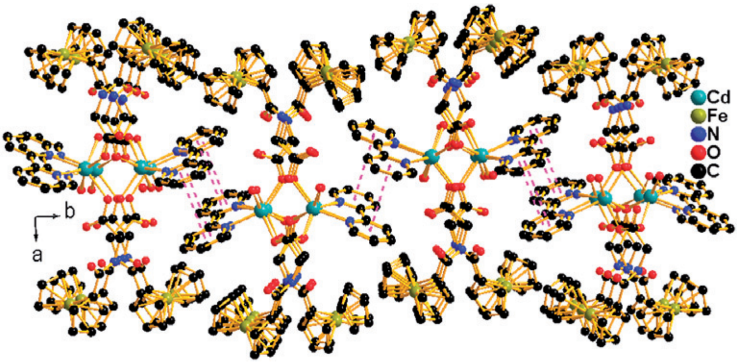

Figure 6. 2-D supramolecular structure of **3** formed from 1-D chains by $\pi \cdots \pi$ stacking interactions. Hydrogen atoms are omitted for clarity.

All C–C–C bond angles of each ferrocene in **1**–**3** are nearly 108°, with the C–C distances of *ca*. 1.4 Å, in accord with those reported in [11, 12, 14, 27]. All ferrocenyl groups are eclipsed with their two cyclopentadienyl rings nearly parallel to each other.

3.3. *Structural discussion*

Comparing the binuclear **2**, 1-D polymer **3**, and mononuclear complex [Cd(phen)(FcCOO)(η^2-FcCOO)(H_2O)] reported previously by our group [28],

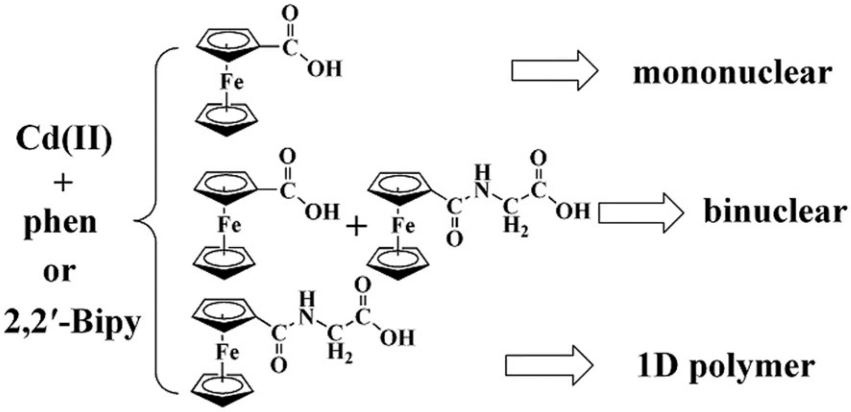

Figure 7. A schematic representation of the stereo-hindrance effect of ferrocenyl groups on the structural difference.

compositions and structures of cadmium(II) complexes with ferrocenylcarboxylate ligands are greatly influenced by the stereo-hindrance of ferrocenyl groups. The ferrocene-containing ligand $FcCOO^-$ in the reported case led to the formation of mononuclear structure, $[Cd(phen)(FcCOO)(\eta^2\text{-}FcCOO)(H_2O)]$. The coexistence of $FcCOO^-$ and $FcCONHCH_2COO^-$ in **2** gave a binuclear structure. However, the use of $FcCONHCH_2COO^-$ alone in **3** produced a 1-D chain structure. These can be attributed to the steric hindrance induced by ferrocenyl groups, which have a strong dependence on the distance between the ferrocenyl and carboxylato groups. The distance in $FcCONHCH_2COO^-$ is much longer than that in $FcCOO^-$, resulting in a much smaller steric hindrance induced by ferrocenyl groups in $FcCONHCH_2COO^-$ than in $FcCOO^-$. As a result, these cadmium(II) complexes have structural variation from mononuclear for $[Cd(phen)(FcCOO)(\eta^2\text{-}FcCOO)(H_2O)]$ with $FcCOO^-$ as the primary ligand to binuclear for **2** with the coexistence of $FcCOO^-$ and $FcCONHCH_2COO^-$ and 1-D polymer for **3** with only $FcCONHCH_2COO^-$ as the ligand, as shown in figure 7.

4. Conclusion

Ferrocenecarboxylate-containing lead(II) and cadmium(II) complexes of **1**–**3** were synthesized and structurally characterized. Complexes **1** and **2** exhibit similar binuclear structures, which are further extended into 1-D chains *via* hydrogen bonding interactions involving guest water molecules. Complex **3** is a 1-D chain structure with two kinds of $FcCONHCH_2COO^-$ ligands arranged regularly along the chain. The structures of the cadmium(II) complexes of $[Cd(phen)(FcCOO)(\eta^2\text{-}FcCOO)(H_2O)]$, **2**, and **3** reveal a variation from mononuclear to binuclear, and 1-D chain, which is ascribed to the stereo-hindrance of ferrocenyl groups.

Supplementary material

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre as Supplementary Publication Nos. CCDC 786033–786035. Copies of the data can be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336 033; Email: deposit@ccdc.cam.ac.uk).

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