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Assembly and Properties of Transition Metal Coordination Polymers Based on Semi-rigid Bis-pyridyl-bis-amide Ligand: Effect of Polycarboxylates on the Dimensionality

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Selected Bond Distances (Å) and Angles (deg) for Complexes **1**–**7**

Complex **1**			
Co(1)–O(1)	2.0491(11)	Co(1)–O(2W)	2.0564(11)
Co(1)–O(1W)	2.1055(11)	Co(1)–O(3W)	2.1407(11)
Co(1)–N(3)	2.1911(12)	Co(1)–N(1)	2.1969(12)
O(1)–Co(1)–O(2W)	176.28(4)	O(1)–Co(1)–O(3W)	92.33(4)
O(1)–Co(1)–O(1W)	92.45(4)	O(2W)–Co(1)–O(3W)	85.68(4)
O(2W)–Co(1)–O(1W)	89.47(4)	O(1W)–Co(1)–O(3W)	175.06(4)
O(1)–Co(1)–N(3)	93.18(5)	O(2W)–Co(1)–N(1)	88.76(4)
O(2W)–Co(1)–N(3)	90.03(4)	O(1W)–Co(1)–N(1)	91.60(4)
O(1W)–Co(1)–N(3)	89.17(4)	O(3W)–Co(1)–N(1)	87.31(4)
O(3W)–Co(1)–N(3)	91.82(4)	N(3)–Co(1)–N(1)	178.56(4)
O(1)–Co(1)–N(1)	88.00(5)		
Complex **2**			
Co(1)–O(3)#1	2.0391(19)	Co(1)–N(2)	2.178(2)
Co(1)–N(1)	2.112(2)	Co(1)–O(2W)	2.2123(19)
Co(1)–O(1)	2.140(2)	Co(1)–O(2)	2.166(2)
O(3)#1–Co(1)–O(1)	159.38(8)	N(1)–Co(1)–O(2W)	89.18(8)
N(1)–Co(1)–O(1)	103.22(8)	O(1)–Co(1)–O(2W)	90.18(8)
O(3)#1–Co(1)–O(2)	98.35(8)	O(2)–Co(1)–O(2W)	83.21(8)
N(1)–Co(1)–O(2)	162.33(9)	N(2)–Co(1)–O(2W)	177.34(8)
O(1)–Co(1)–O(2)	61.05(7)	O(3)#1–Co(1)–N(2)	89.58(8)
N(1)–Co(1)–N(2)	89.93(9)	O(1)–Co(1)–N(2)	92.47(8)
O(2)–Co(1)–N(2)	98.34(8)	O(3)#1–Co(1)–O(2W)	88.05(7)
O(3)#1–Co(1)–N(1)	97.30(9)		
Symmetry transformations used to generate equivalent atoms: #1 – x, y + 1/2, – z + 1/2			
Complex **3**			
Co(1)–O(5)	1.9715(18)	Co(1)–O(3)#2	2.0857(17)

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Co(1)–O(2)#1	1.9828(17)	Co(1)–O(4)#2	2.290(2)
Co(1)–N(1)	2.0688(19)	Co(2)–O(1)	2.1021(17)
Co(2)–O(4W)#3	2.059(3)	Co(2)–O(1)#3	2.1021(17)
Co(2)–O(4W)	2.059(3)	Co(2)–O(3W)#3	2.148(2)
Co(2)–O(3W)	2.148(2)	O(5)–Co(1)–O(2)#1	104.73(7)
O(5)–Co(1)–N(1)	96.96(7)	O(5)–Co(1)–O(4)#2	161.61(8)
O(2)#1–Co(1)–N(1)	114.92(7)	O(2)#1–Co(1)–O(4)#2	85.58(7)
O(5)–Co(1)–O(3)#2	102.75(7)	N(1)–Co(1)–O(4)#2	92.21(8)
O(2)#1–Co(1)–O(3)#2	125.94(7)	O(3)#2–Co(1)–O(4)#2	59.20(8)
N(1)–Co(1)–O(3)#2	106.70(7)	O(4W)#3–Co(2)–O(4W)	180.00
O(4W)#3–Co(2)–O(1)	93.55(8)	O(4W)#3–Co(2)–O(1)#3	86.45(8)
O(4W)–Co(2)–O(1)	93.55(8)	O(4W)–Co(2)–O(1)#3	93.55(8)
O(1)–Co(2)–O(1)#3	180.00	O(4W)#3–Co(2)–O(3W)	91.71(9)
O(4W)#3–Co(2)–O(3W)#3	91.71(9)	O(4W)–Co(2)–O(3W)	91.71(9)
O(4W)–Co(2)–O(3W)#3	91.71(19)	O(1)–Co(2)–O(3W)	95.28(8)
O(1)–Co(2)–O(3W)#3	95.29(8)	O(1)#3–Co(2)–O(3W)	84.71(8)
O(1)#3–Co(2)–O(3W)#3	95.29(8)	O(3W)#3–Co(2)–O(3W)	180.00

Symmetry transformations used to generate equivalent atoms: #1 x + 1, y, z; #2 x + 1/2, – y + 1/2, z – 1/2; #3 – x – 2, – y, – z

Complex **4**

Co(1)–O(1)	1.906(3)	Co(1)–O(3B)#2	1.985(5)
Co(1)–O(3A)#1	1.985(5)	Co(1)–N(1)#3	2.044(2)
Co(1)–N(1)	2.044(2)	O(1)–Co(1)–N(1)	116.29(8)
O(1)–Co(1)–O(3A)#1	106.53(2)	O(3B)#1–Co(1)–N(1)#3	93.20(17)
O(1)–Co(1)–O(3B)#1	106.53(2)	O(3B)#2–Co(1)–N(1)#3	119.76(18)
O(1)–Co(1)–O(3B)#2	106.53(2)	O(1)–Co(1)–N(1)#3	116.29(8)
N(1)#3–Co(1)–N(1)	102.86(9)	O(3B)#1–Co(1)–N(1)	119.76(18)
O(3B)#1–Co(1)–O(3B)#2	32.72(2)	O(3B)#2–Co(1)–N(1)	93.20(17)

Symmetry transformations used to generate equivalent atoms: #1 x – 1/2, y, – z + 1/2; #2 x – 1/2, – y + 3/2, – z + 1/2; #3 x, – y + 3/2, z

Complex **5**

Cu(1)–O(1)	1.9202(14)	Cu(1)–O(3)#1	1.9671(13)
Cu(1)–N(1)	2.0433(17)	Cu(1)–N(4)#2	2.0667(16)
Cu(1)–O(6)#3	2.4375(16)	O(1)–Cu(1)–O(3)#1	167.56(7)
O(1)–Cu(1)–N(1)	92.21(7)	O(3)#1–Cu(1)–N(1)	89.17(6)
O(1)–Cu(1)–N(4)#2	89.33(6)	O(3)#1–Cu(1)–N(4)#2	87.39(6)
N(1)–Cu(1)–N(4)#2	170.71(7)	O(1)–Cu(1)–O(6)#3	105.72(6)
O(3)#1–Cu(1)–O(6)#3	86.26(6)	N(1)–Cu(1)–O(6)#3	98.97(6)
N(4)#2–Cu(1)–O(6)#3	89.42(6)		

Symmetry transformations used to generate equivalent atoms: #1 x + 1, y, z; #2 x – 1, – y + 1/2, z + 1/2; #3 – x + 2, y – 1/2, – z + 3/2

Complex **6**

Cu(1)–O(1)	1.9430(15)	Cu(1)–O(1)#1	1.9430(15)

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Cu(1)–N(3)	2.049(2)	Cu(1)–N(3)#1	2.049(2)
Cu(2)–O(3)	1.9531(19)	Cu(2)–O(3)#2	1.9531(19)
Cu(2)–N(1)#2	2.004(2)	O(1)–Cu(1)–O(1)#1	180.00
O(1)–Cu(1)–N(3)	90.73(7)	O(1)#1–Cu(1)–N(3)	89.28(7)
O(1)–Cu(1)–N(3)#1	89.28(7)	O(1)#1–Cu(1)–N(3)#1	90.73(7)
N(3)–Cu(1)–N(3)#1	180.00	O(3)–Cu(2)–O(3)#2	180.00
O(3)–Cu(2)–N(1)#2	93.41(8)	O(3)#2–Cu(2)–N(1)#2	86.59(8)
O(3)–Cu(2)–N(1)	86.59(9)	O(3)#2–Cu(2)–N(1)	93.41(8)
N(1)#2–Cu(2)–N(1)	180.00		

Symmetry transformations used to generate equivalent atoms: #1 – x + 1/2, – y + 1/2, – z; #2 – x + 1/2, – y – 1/2, – z

Complex **7**

Cu(1)–O(18)	1.929(5)	Cu(1)–O(8)#1	1.947(6)
Cu(1)–N(2)	2.038(8)	Cu(1)–N(8)	2.062(9)
Cu(1)–O(4W)	2.249(7)	Cu(1)–O(11)	2.758(8)
Cu(2)–O(5)	1.909(5)	Cu(2)–O(7)	1.926(5)
Cu(2)–N(3)#2	2.047(9)	Cu(2)–N(6)	2.051(8)
Cu(2)–O(3W)	2.455(8)	O(18)–Cu(1)–O(8)#1	174.2(3)
O(18)–Cu(1)–N(2)	90.6(3)	O(8)#1–Cu(1)–N(2)	90.1(3)
O(18)–Cu(1)–N(8)	88.9(3)	O(8)#1–Cu(1)–N(8)	91.6(3)
N(2)–Cu(1)–N(8)	167.5(4)	O(18)–Cu(1)–O(4W)	92.0(2)
O(8)#1–Cu(1)–O(4W)	82.3(3)	N(2)–Cu(1)–O(4W)	94.4(3)
N(8)–Cu(1)–O(4W)	98.1(3)	O(5)–Cu(2)–O(7)	172.3(3)
O(5)–Cu(2)–N(3)#2	87.5(3)	O(7)–Cu(2)–N(3)#2	93.0(3)
O(5)–Cu(2)–N(6)	90.2(3)	O(7)–Cu(2)–N(6)	88.1(3)
N(3)#2–Cu(2)–N(6)	170.8(4)		

Symmetry transformations used to generate equivalent atoms: #1 x, y, z + 1; #2 x + 2, y + 1, z

Table S2. Hydrogen–Bonding Geometry (Å, °) for Complexes **1** and **6**.

D–H···A	D–H	H···A	D···A	D–H···
	Complex **1**			
O(1W)–H(1WA)···O(6)[a]	0.85	1.91	2.7548(16)	173
N(4)–H(4A)···O(4W)	0.86	2.19	2.9860(17)	154
O(4W)–H4WA···O3[b]	0.85	1.93	2.7468(13)	160
	Complex **6**			
N(2)–H(2A)···O(2)[a]	0.86	1.93	2.774(3)	167
N(4)–H(4B)···O(6)[b]	0.86	2.08	2.928(3)	169
	Complex **7**			
O(3)–H(3A)···O(14)[a]	0.82	1.801	2.570	155.46
O(19)–H(19A)···O(16)[b]	0.82	1.831	2.588	152.9

Symmetry code for **1**: (a) x, – y + 1, – 1/2 + z; (b) – x + 3/2, – y + 3/2, – z + 1; for **6**: (a) – 1/2 + x, – 1/2 + y, z; (b) x, 1 + y, z; for **7**: (a) x + 1, y, z; (b) x – 1, y, z.

Fig. S1. The 1D sinusoid-like chain in **1**.

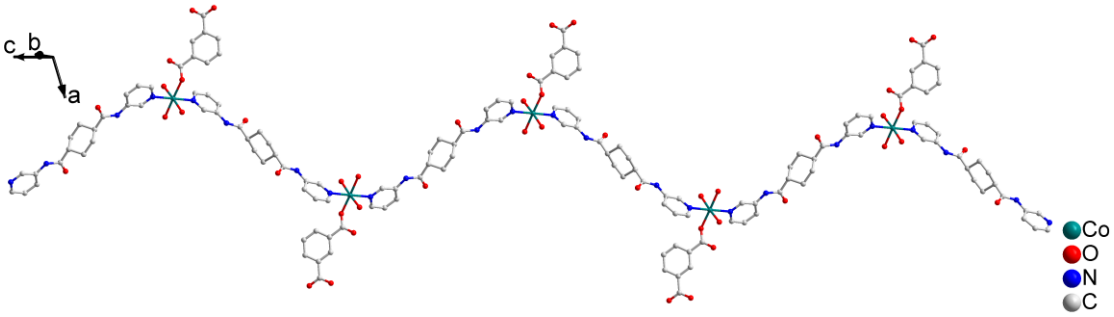

Fig. S2. The 3D supramolecular framework based on the 2D supramolecular networks by hydrogen bonding interactions of complex **1**. The hydrogen atoms are omitted for clarity.

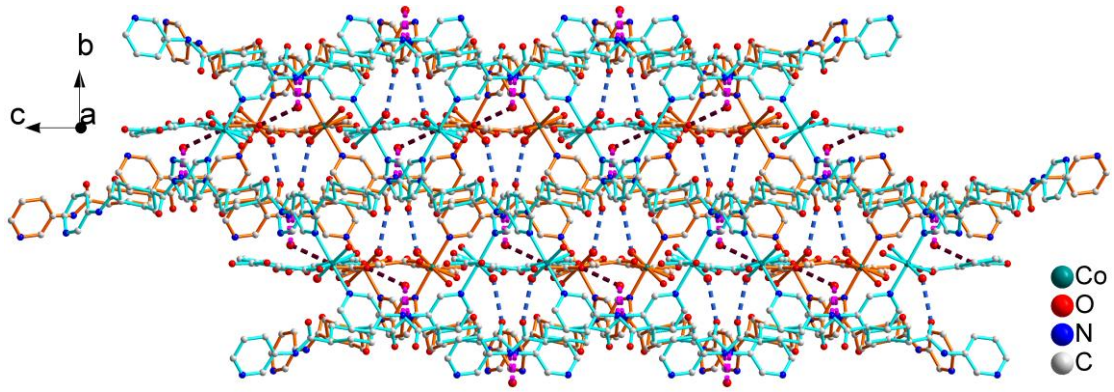

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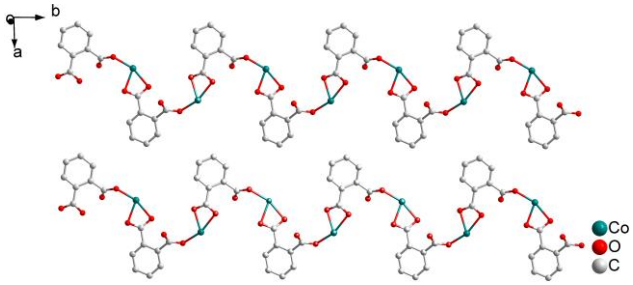
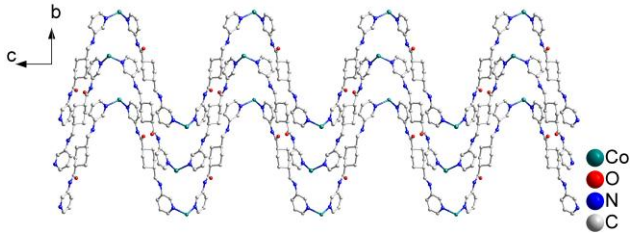
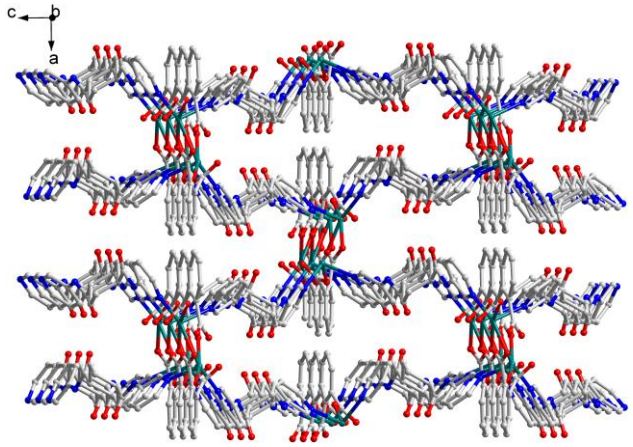
Fig. S3. (a) The 1D chain based on the Co^{II} ions and the 1,2-BDC carboxylate ligand along b direction. (H atoms are omitted for clarity). (b) 1D chain based on the Co^{II} ions and the **3-bpcd** ligands along c direction in complex **2**. (c) The 3D framework of **2** based on the 2D layer and the 1,2-BDC carboxylate.



(a)

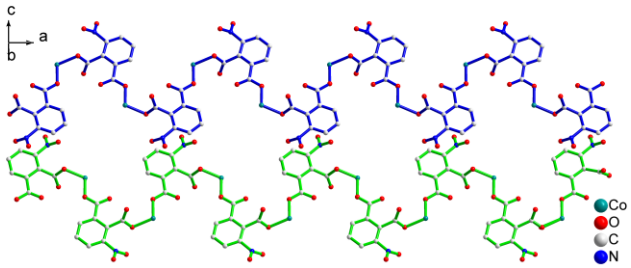


(b)

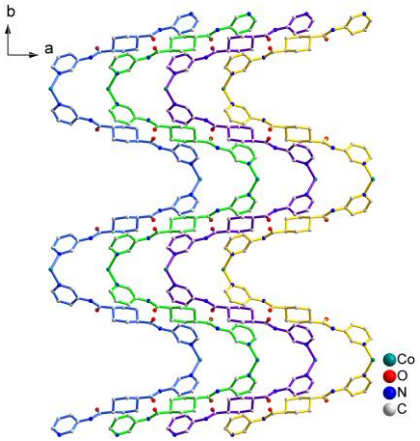


(c)

Fig. S4. (a) The 1D chain based on the Co^{II} ions and the NPH ligands. (b) 1D chain based on the Co^{II} ions and the **3-bpcd** ligands in complex **4**. (H atoms are omitted for clarity).



(a)



(b)

Fig. S5. The 1D Cu-1,3-BDC chain of complex **5**.

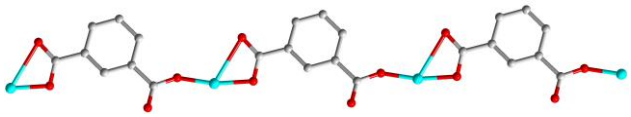


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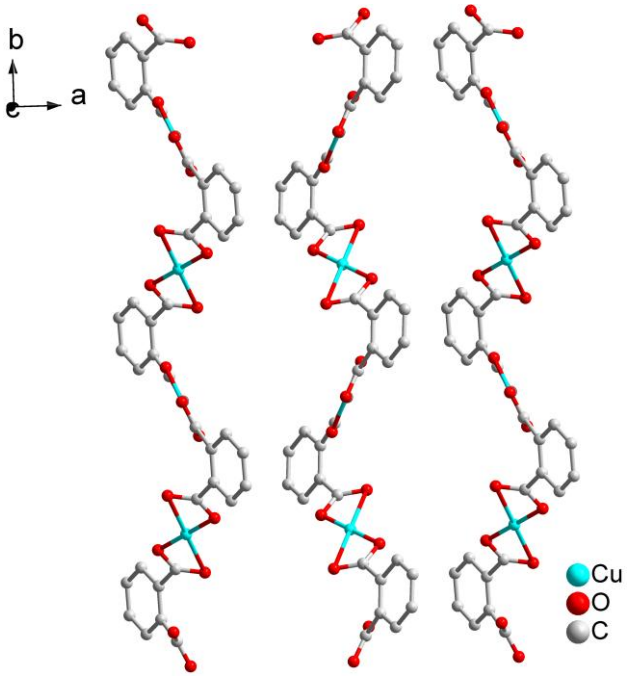
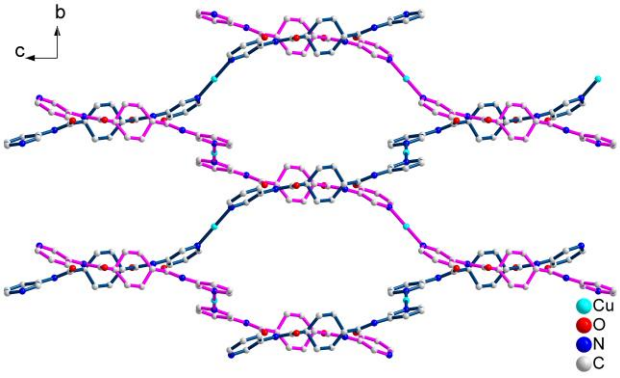
Fig. S6. (a) The 1D chain based on the Cu^{II} ions and the 1,2-BDC ligands. (b) 1D chains based on the Cu^{II} ions and the **3-bpcd** ligands in complex **6**. (H atoms are omitted for clarity).



(a)



(b)

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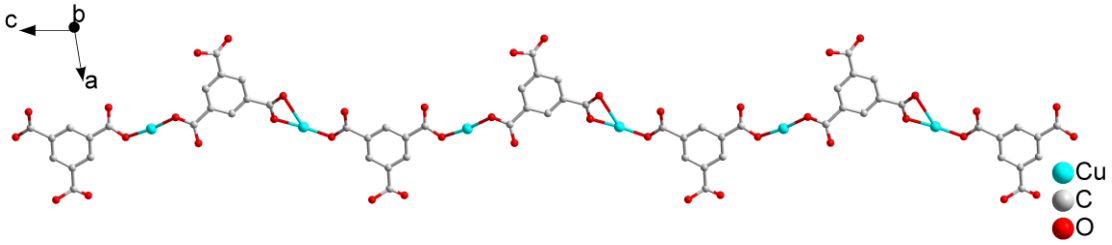
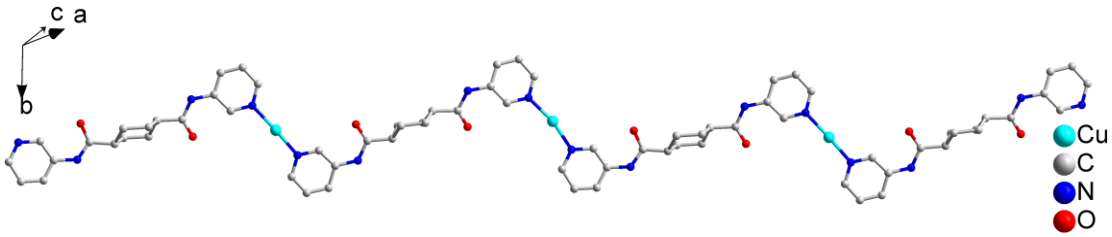
Fig. S7. (a) The 1D chain based on the Cu^{II} ions and the 1,3,5-HBTC ligands. (b) 1D chain based on the Cu^{II} ions and the **3-bpcd** ligands in complex **7**. (H atoms are omitted for clarity).



(a)



(b)

Figure S8. The TG curves of complexes **1**–**7**.

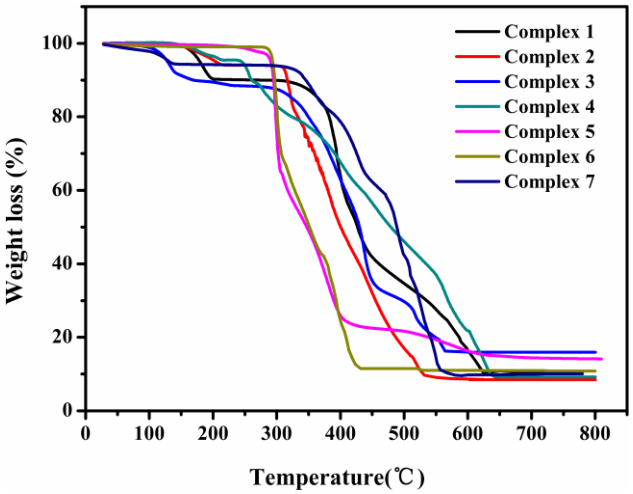


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Fig. S9. Cyclic voltammogram of **2**–CPE (+900 to –800mV) in 1 M H_2SO_4 solution for complex **2**. Scan rate: 100 mVs^{-1}.

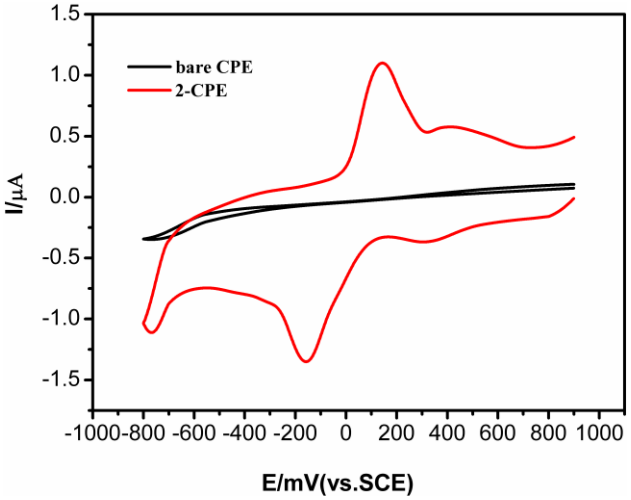

Fig. S10. Cyclic voltammogram of **7**–CPE (+400 to –400mV) in 1 M H_2SO_4 solution for complex **7**. Scan rate: 100 mVs^{-1}.