A Series of Organic–inorganic Hybrid Materials Consisting of Flexible Organic Amine Modified Polyoxomolybdates: Synthesis, Structures, and Properties

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Table S1 Selected bond lengths and angles for complexes **1**–**7**.

Complex 1			
Zn1–O1W	1.917(6)	Zn2–N5	2.224(7)
Zn1–N1	2.245(7)	Zn2–N6	2.027(7)
Zn1–N2	2.081(8)	Zn2–N7	2.057(7)
Zn1–N3	2.050(8)	Zn2–N8	2.066(8)
Zn1–N4	2.083(8)	Zn2–O11	1.977(5)
O1W–Zn1–N1	170.6(3)	N6–Zn2–N5	80.1(3)
O1W–Zn1–N2	98.8(3)	N6–Zn2–N7	119.9(3)
O1W–Zn1–N3	109.7(3)	N6–Zn2–N8	118.6(3)
O1W–Zn1–N4	97.6(3)	N7–Zn2–N5	80.1(3)
N2–Zn1–N1	78.0(3)	N7–Zn2–N8	112.7(3)
N2–Zn1–N4	123.7(3)	N8–Zn2–N5	80.0(3)
N3–Zn1–N1	79.6(3)	O11–Zn2–N5	175.8(3)
N3–Zn1–N2	106.1(3)	O11–Zn2–N6	96.4(3)
N3–Zn1–N4	117.9(3)	O11–Zn2–N7	99.9(2)
N4–Zn1–N1	77.3(3)	O11–Zn2–N8	103.8(3)
Complex 2			
Zn1–O1	1.998(2)	Zn1–N4	2.065(3)
Zn1–N3	2.046(3)	Zn1–N1	2.219(3)

Zn1–N2	2.049(3)		
O1–Zn1–N3	105.38(10)	N2–Zn1–N4	121.28(11)
O1–Zn1–N2	99.42(11)	O1–Zn1–N1	174.10(9)
N3–Zn1–N2	116.94(11)	N3–Zn1–N1	80.32(10)
O1–Zn1–N4	97.84(10)	N2–Zn1–N1	78.97(11)
N3–Zn1–N4	111.45(11)	N4–Zn1–N1	78.39(10)
Complex 3			
Co1–O1	1.9695(19)	Co1–N3	2.065(2)
Co1–N4	2.045(2)	Co1–N1	2.208(2)
Co1–N2	2.060(2)		
O1–Co1–N4	105.52(9)	N2–Co1–N3	121.02(10)
O1–Co1–N2	100.27(9)	O1–Co1–N1	175.43(9)
N4–Co1–N2	115.97(10)	N4–Co1–N1	78.97(9)
O1–Co1–N3	99.77(9)	N2–Co1–N1	78.22(9)
N4–Co1–N3	110.80(9)	N3–Co1–N1	77.56(9)
Complex 4			
Ni1–O1	2.025(3)	Ni1–N3	2.087(4)
Ni1–N4	2.059(4)	Ni1–N1	2.096(4)
Ni1–N2	2.060(4)	Ni1–O1W	2.138(3)
O1–Ni1–N4	97.76(14)	N2–Ni1–N1	81.25(15)
O1–Ni1–N2	99.49(14)	N3–Ni1–N1	82.74(16)
N4–Ni1–N2	162.74(16)	O1–Ni1–O1W	90.03(13)
O1–Ni1–N3	94.02(14)	N4–Ni1–O1W	89.17(14)
N4–Ni1–N3	88.86(15)	N2–Ni1–O1W	90.13(14)
N2–Ni1–N3	90.62(15)	N3–Ni1–O1W	175.70(14)
O1–Ni1–N1	176.70(15)	N1–Ni1–O1W	93.19(14)
N4–Ni1–N1	81.58(15)		
Complex 5			
Ni1-N4	2.053(9)	Ni2-O2	2.002(7)
Ni1-N9	2.055(8)	Ni2-N7	2.046(8)
Ni1-N2	2.058(8)	Ni2-N6	2.067(10)
Ni1-N3	2.082(8)	Ni2-N8	2.068(10)
Ni1-N1	2.094(9)	Ni2-N5	2.112(9)
Ni1-O1	2.100(7)		
N4-Ni1-N9	98.2(3)	O2-Ni2-N7	89.0(3)
N4-Ni1-N2	162.1(4)	O2-Ni2-N6	94.7(4)
N9-Ni1-N2	97.3(3)	N7-Ni2-N6	96.5(4)
N4-Ni1-N3	87.1(3)	O2-Ni2-N8	101.5(4)
N9-Ni1-N3	104.9(3)	N7-Ni2-N8	89.4(4)
N2-Ni1-N3	97.5(3)	N6-Ni2-N8	162.9(4)
N4-Ni1-N1	81.8(3)	O2-Ni2-N5	171.1(3)
N9-Ni1-N1	171.7(4)	N7-Ni2-N5	83.1(3)
N2-Ni1-N1	81.6(4)	N6-Ni2-N5	82.3(4)
N3-Ni1-N1	83.4(4)	N8-Ni2-N5	82.5(4)

N4-Ni1-O1	85.6(3)	O2-Ni2-O1W	91.8(3)
N9-Ni1-O1	79.6(3)	N7-Ni2-O1W	175.3(4)
N2-Ni1-O1	88.4(3)	N6-Ni2-O1W	88.0(4)
N3-Ni1-O1	172.0(3)	N8-Ni2-O1W	85.9(3)
N1-Ni1-O1	92.1(3)	N5-Ni2-O1W	96.4(3)
Complex 6			
Cu1–O1	1.930(2)	Cu1–N1	2.053(3)
Cu1–N4	2.037(3)	Cu1–N3	2.089(3)
Cu1–N2	2.047(3)		
O1–Cu1–N4	177.07(11)	N2–Cu1–N1	127.06(11)
O1–Cu1–N2	97.81(11)	O1–Cu1–N3	100.38(10)
N4–Cu1–N2	82.44(11)	N4–Cu1–N3	82.11(11)
O1–Cu1–N1	96.27(10)	N2–Cu1–N3	114.83(11)
N4–Cu1–N1	81.31(11)	N1–Cu1–N3	112.24(11)
Complex 7			
Cu1–O1	1.917(3)	Cu2–N5	2.065(4)
Cu1–N1	2.030(4)	Cu2–N6	2.041(4)
Cu1–N2	2.079(5)	Cu2–N7	2.067(4)
Cu1–N3	2.071(5)	Cu2–N8	2.034(4)
Cu1–N4	2.021(4)	Cu2–O21	1.955(3)
O1–Cu1–N4	178.44(16)	O21–Cu2–N8	177.68(16)
O1–Cu1–N1	94.98(16)	O21–Cu2–N6	96.56(15)
N4–Cu1–N1	83.52(18)	N8–Cu2–N6	82.25(16)
O1–Cu1–N3	98.74(17)	O21–Cu2–N7	100.21(15)
N4–Cu1–N3	82.3(2)	N8–Cu2–N7	82.11(16)
N1–Cu1–N3	117.5(2)	N6–Cu2–N7	118.69(16)
O1–Cu1–N2	98.79(17)	O21–Cu2–N5	97.60(14)
N4–Cu1–N2	81.7(2)	N8–Cu2–N5	81.38(15)
N1–Cu1–N2	123.46(19)	N6–Cu2–N5	121.09(17)
N3–Cu1–N2	114.06(19)	N7–Cu2–N5	114.38(16)

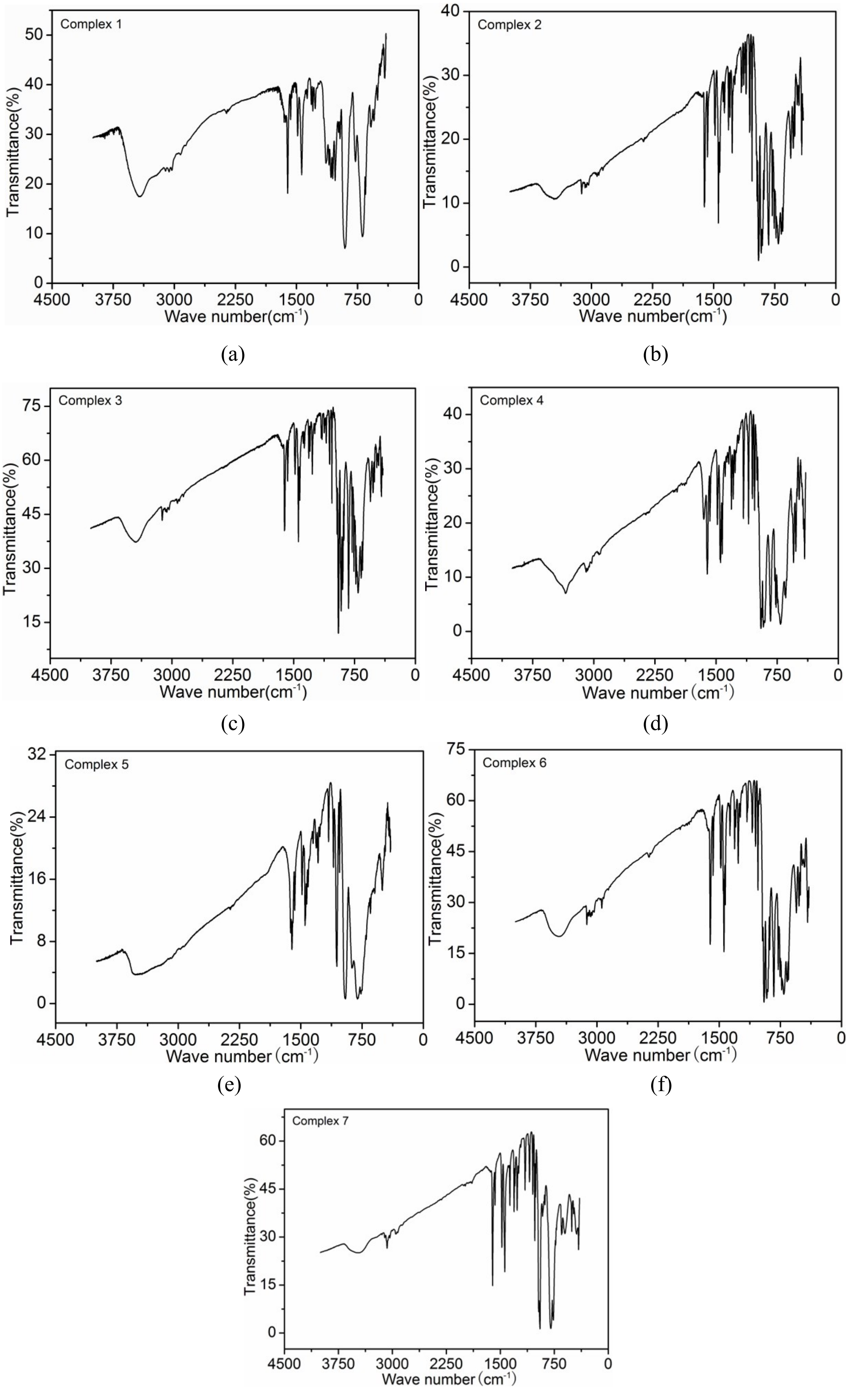
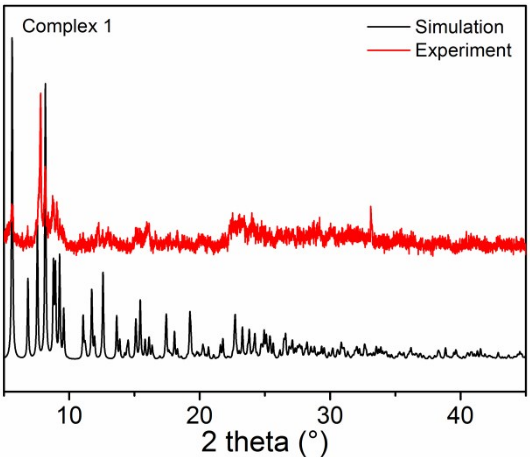
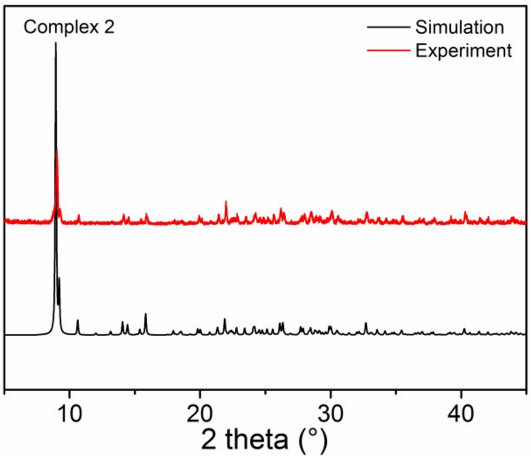


Fig. S1 The IR spectra of complexes **1**–**7**.


Complex 1
Simulation
Experiment
10
20
30
40
2 theta (°)

(a)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Simulation
Experiment
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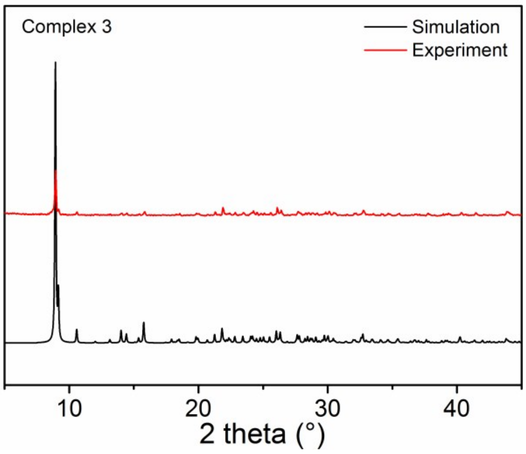
2 theta (°)

(b)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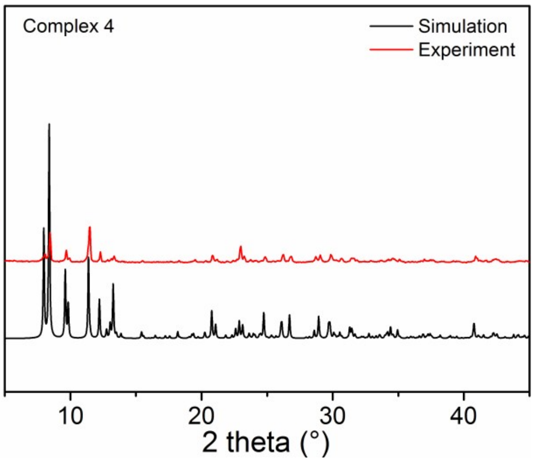
Simulation
Experiment
10
20
30
40
2 theta (°)

(c)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Simulation
Experiment
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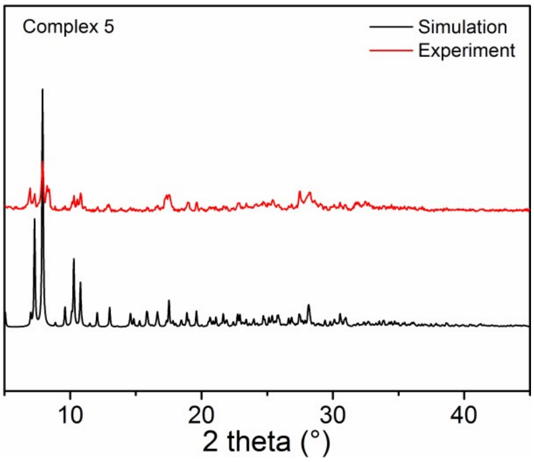
20
30
40
2 theta (°)

(d)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Simulation
Experiment
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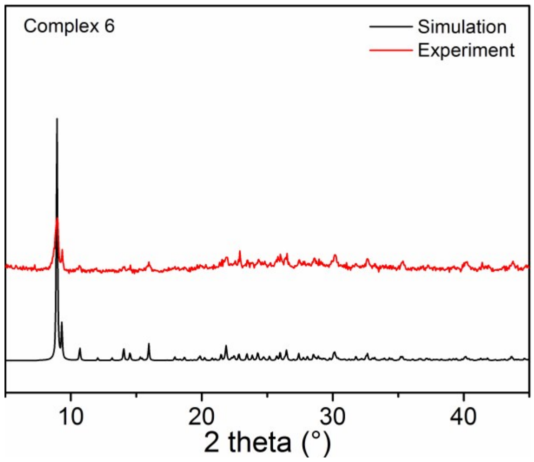
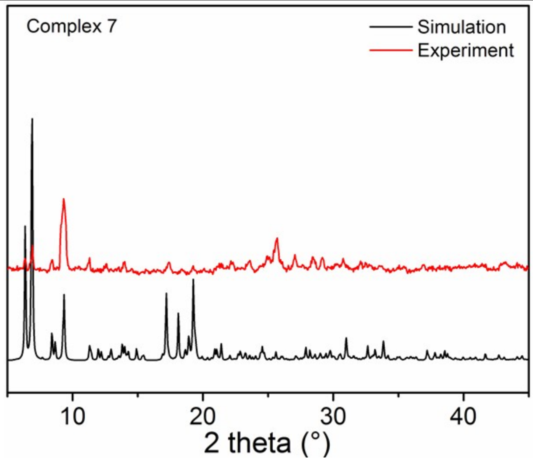
20
30
40
2 theta (°)

(e)

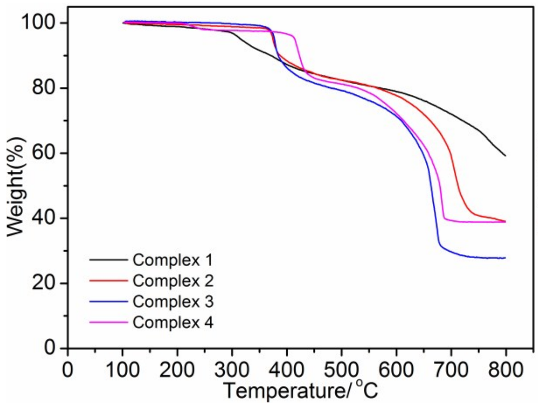

Complex 6
Simulation
Experiment
10
20
30
40
2 theta (°)

(f)

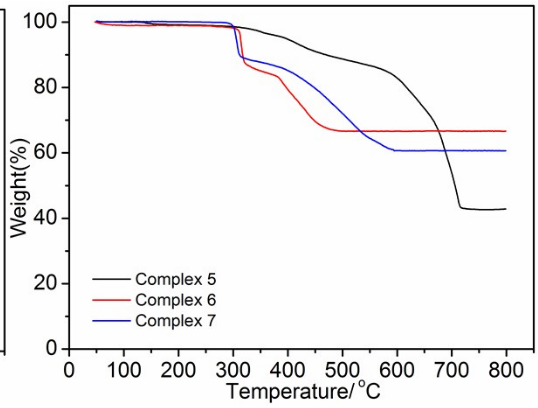


(g)

Fig. S2 The Powder X–ray diffraction pattern of complexes **1**–**7**.



(a)



(b)

Fig. S3 The TG curves of complexes **1**–**7**.

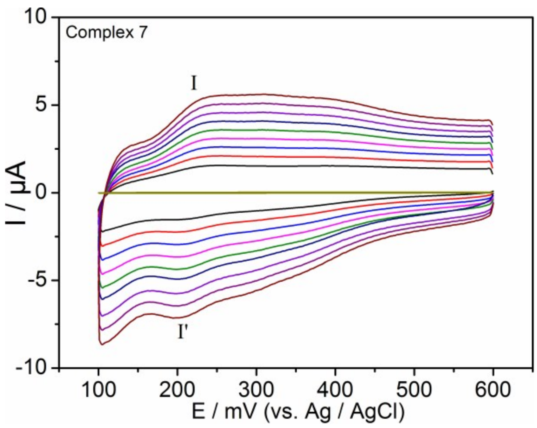
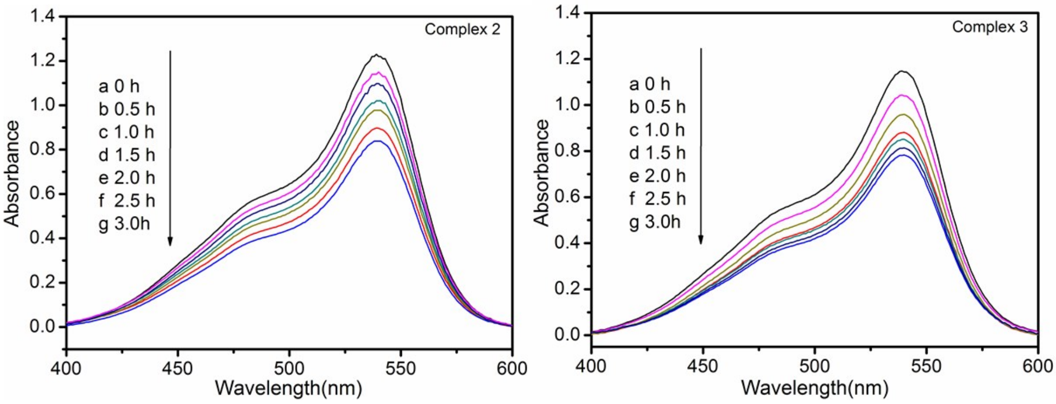


Fig. S4 Cyclic voltammograms of **7**-CPE in 0.5 M Na_2SO_4 + 0.1 M H_2SO_4 aqueous solution at distinct scanning rates (from inside to out: 50, 100, 150, 200, 250, 300, 350, 400, 450, 500 mV s^{-1}) , respectively.



(a) (b)

Fig. S5 Photocatalytic activities of complexes **2** (a) and **3** (b).