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Various Amide-derived Ligands Induced Five Octamolybdate−based Metal-organic Complexes: Synthesis, Structure, Electrochemical Sensing and Photocatalytic Properties

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Table S1 Selected bond distances (Å) and angles (°) for complexes **1**-**5**.

Complex **1**			
Co(1)-O(2)	2.089(10)	Co(1)-O(3)#1	2.023(8)
Co(1)-O(1)	2.045(9)	Co(1)-N(5)#1	2.045(10)
Co(1)-N(1)	2.027(11)		
O(3)#1-Co(1)-O(2)	112.6(4)	O(3)#1-Co(1)-O(1)	159.0(4)
O(3)#1-Co(1)-N(5)#1	81.4(4)	O(3)#1-Co(1)-N(1)	96.0(4)
O(1)-Co(1)-O(2)	88.4(4)	N(5)#1-Co(1)-O(2)	93.9(4)
N(5)#1-Co(1)-O(1)	97.2(4)	N(1)-Co(1)-O(2)	99.2(4)
N(1)-Co(1)-O(1)	80.4(4)	N(1)-Co(1)-N(5)#1	166.6(5)
Symmetry code for **1**:	#1 x-1,y-1,z		

Complex **2**			
Ni(1)-O(4)	2.115(10)	Ni(1)-O(1W)	2.051(10)
Ni(1)-O(9)#1	2.080(11)	Ni(1)-N(2)	2.046(15)
Ni(1)-N(3)#1	2.038(13)	Ni(1)-O(2W)	2.056(14)
O(1W)-Ni(1)-O(4)	91.8(4)	O(1W)-Ni(1)-O(9)#1	174.0(5)
O(1W)-Ni(1)-O(2W)	85.3(5)	O(9)#1-Ni(1)-O(4)	87.1(4)
N(2)-Ni(1)-O(4)	79.6(5)	N(2)-Ni(1)-O(1W)	92.5(5)
N(2)-Ni(1)-O(9)#1	93.2(5)	N(2)-Ni(1)-O(2W)	168.9(6)
N(3)#1-Ni(1)-O(4)	165.7(5)	N(3)#1-Ni(1)-O(1W)	102.3(5)
N(3)#1-Ni(1)-O(9)#1	79.2(5)	N(3)#1-Ni(1)-N(2)	97.0(5)
N(3)#1-Ni(1)-O(2W)	94.0(6)	O(2W)-Ni(1)-O(4)	89.7(6)
O(2W)-Ni(1)-O(9)#1	88.8(5)		
Symmetry code for **2**:	#1 x-1/2,-y+1/2,z-1/2		

Complex **3**			
Co(1)-O(4)#1	2.185(2)	Co(1)-O(8)	2.086(2)
Co(1)-O(11)	2.116(3)	Co(1)-N(3)	2.100(3)
Co(1)-N(22)#1	2.091(4)	Co(1)-O(18)	2.070(3)
O(8)-Co(1)-O(4)#1	91.97(10)	O(8)-Co(1)-O(11)	174.86(12)
O(8)-Co(1)-N(3)	103.41(11)	O(8)-Co(1)-N(22)#1	91.48(11)
O(11)-Co(1)-O(4)#1	86.79(10)	N(3)-Co(1)-O(4)#1	164.02(11)
N(3)-Co(1)-O(11)	78.26(11)	N(22)#1-Co(1)-O(4)#1	77.86(11)
N(22)#1-Co(1)-O(11)	93.13(12)	N(22)#1-Co(1)-N(3)	97.16(13)
O(18)-Co(1)-O(4)#1	90.84(12)	O(18)-Co(1)-O(8)	86.78(12)
O(18)-Co(1)-O(11)	88.25(13)	O(18)-Co(1)-N(3)	94.29(14)
O(18)-Co(1)-N(22)#1	168.51(13)		
Symmetry code for **3**:	#1 x-1/2,-y+3/2,z-1/2		

Complex **4**			
Zn(1)-O(5)	2.1052(19)	Zn(1)-O(11)	2.125(2)
Zn(1)-N(2)	2.113(3)	Zn(1)-O(5)#1	2.1052(19)
Zn(1)-O(11)#1	2.125(2)	Zn(1)-N(2)#1	2.113(3)
O(5)-Zn(1)-O(5)#1	180.0	O(5)-Zn(1)-O(11)	88.33(8)
O(5)#2-Zn(1)-O(11)	91.67(8)	O(5)-Zn(1)-N(2)	78.67(8)
O(5)#1-Zn(1)-N(2)	101.33(8)	O(11)-Zn(1)-O(11)#1	180.00(11)
N(2)-Zn(1)-O(11)	92.71(9)	N(2)-Zn(1)-O(11)#1	87.29(9)
N(2)-Zn(1)-N(2)#1	180.00(8)		
Symmetry code for **4**:	#1 -x+1,-y+1,-z+1		

Complex **5**			
Co(1)-O(8)	2.062(7)	Co(1)-O(9)	2.116(7)
Co(1)-N(1)	2.098(9)	Co(1)-O(8)#1	2.062(7)
Co(1)-O(9)#1	2.116(7)	Co(1)-N(1)#1	2.098(9)

O(8)#1-Co(1)-O(8)	180.0	O(8)-Co(1)-O(9)#1	88.6(3)
O(8)-Co(1)-O(9)	91.4(3)	O(8)-Co(1)-N(1)	86.8(3)
O(8)-Co(1)-N(1)#1	93.2(3)	O(9)#1-Co(1)-O(9)	180.0
N(1)-Co(1)-O(9)#1	102.0(3)	N(1)-Co(1)-O(9)	78.0(3)
N(1)#1-Co(1)-N(1)	180.0		

Symmetry code for **5**: #1-x+1,-y+1,-z+1

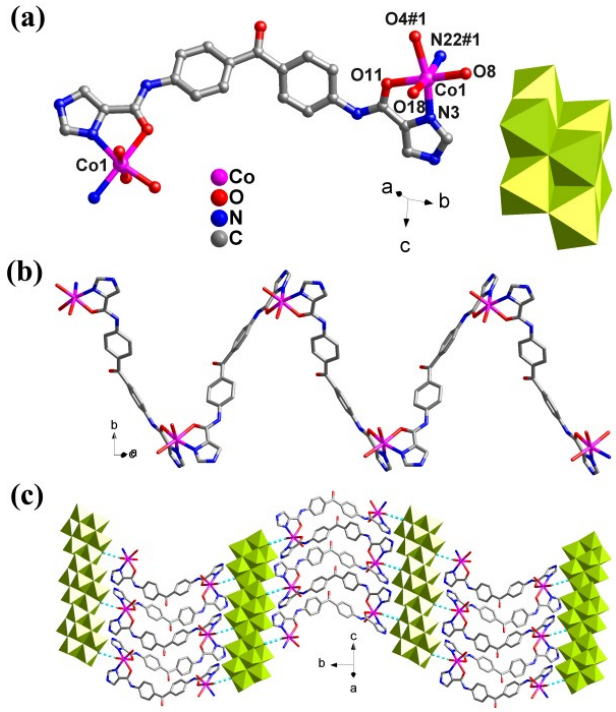

Fig. S1 (a) View of the coordination environment of the Co(II) ion and Mo_8 anion. (b) View of the 1D wave−like Co−L^2 chain. (c) View of the 2D supramolecular structure of **3**.

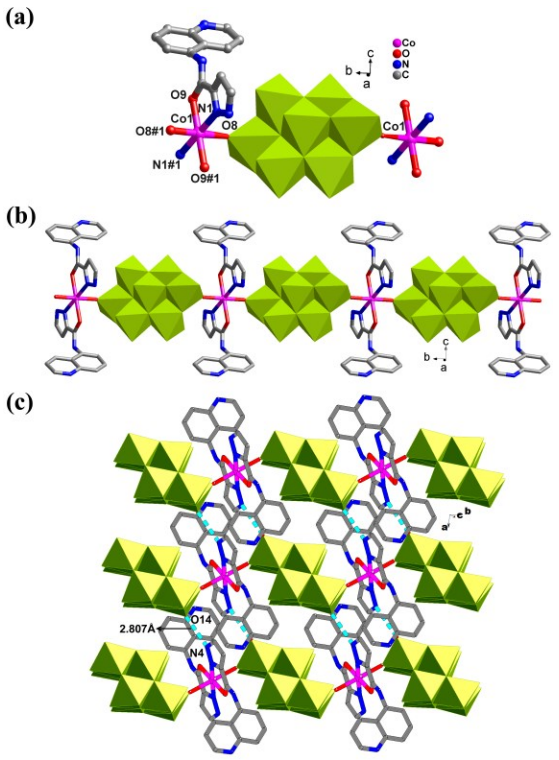

Fig. S2 (a) View of the coordination environment around the Co(II) ion and Mo_8 anion. (b) View of the 1D fence type chain. (c) View of the 2D supramolecular structure.

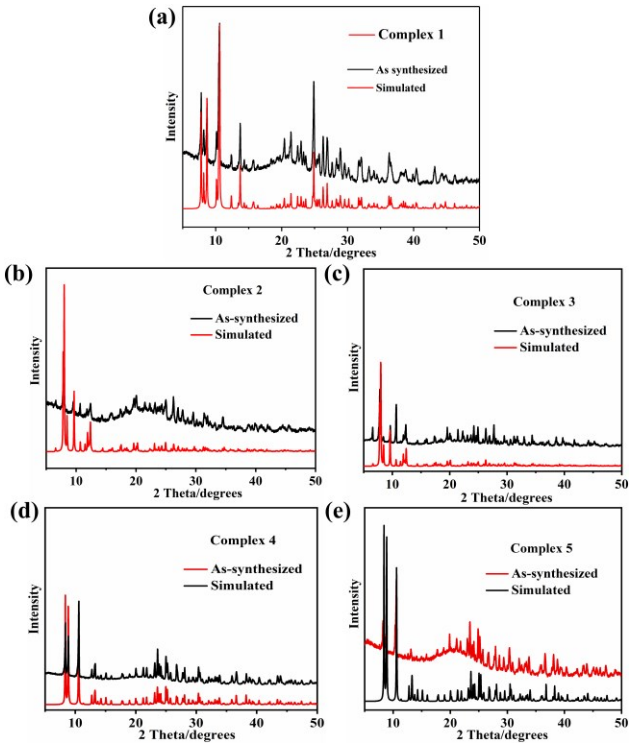

Fig. S3 PXRD patterns of complexes **1-5**.

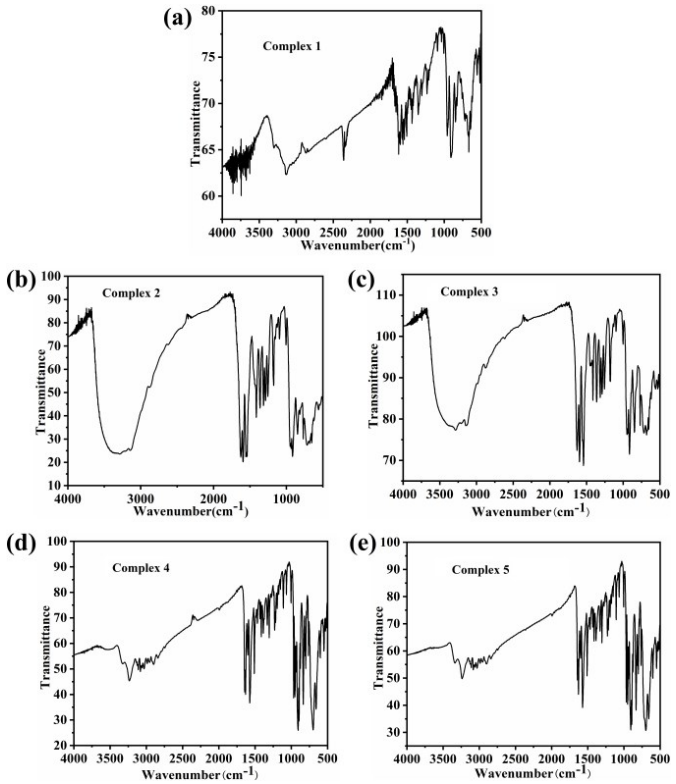

Fig. S4 The IR spectra of complexes **1**-**5**.

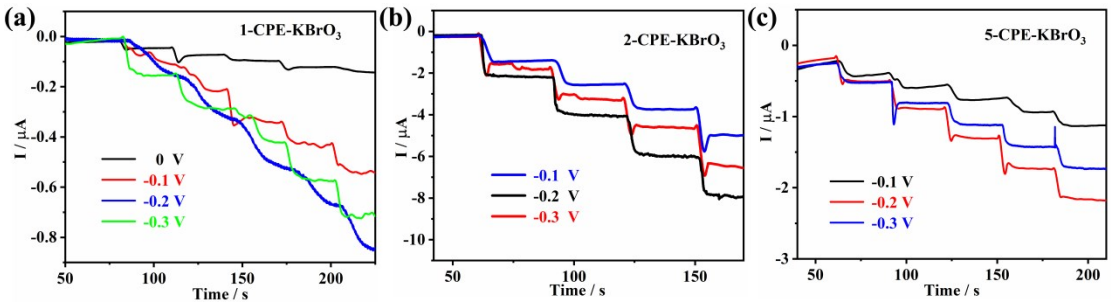

Fig. S5 Amperometric response of **1**-, **2**-, **5**-CPEs at different potentials from -0.3 V to 0 V with successive additions of bromate into electrolyte solution.

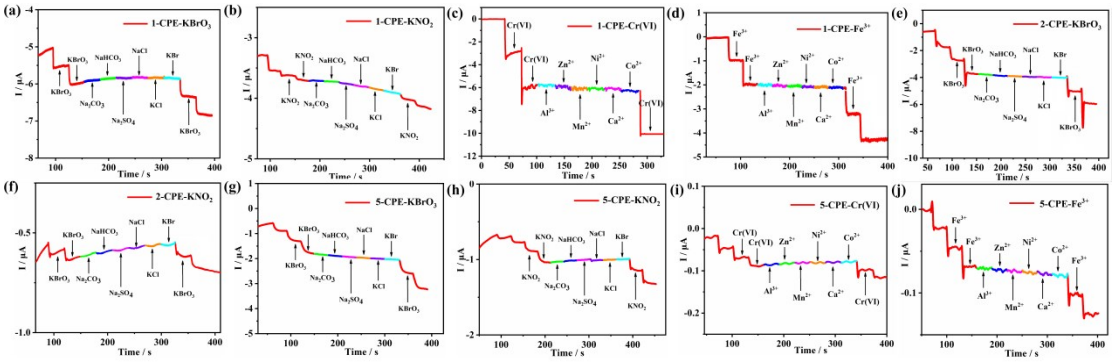

Fig. S6 Amperometric response of **1**-CPE for bromate (a), nitrite (b),Cr(VI) (c) and Fe(Ⅲ) (d) ions and potential interference substances; Amperometric response of **2**-CPE for bromate (e), nitrite (f) and potential interference substances; Amperometric response of **5**-CPE for bromate (g), nitrite (h), Cr(VI) (i), Fe(Ⅲ) (j) ions and potential interference substances.

Table S2 Parameters for bromate, nitrite, Cr(VI) and Fe(Ⅲ) ions detections using **1**-, 2- ,**5**-CPEs.

Material		**1**-CPE	**2**-CPE	**5**-CPE
Detection limit (μmol L^{-1})	$KBrO_3$	1503	25.4	24
	KNO_2	7598	101	200
	Cr(VI)	9.44	—	0.7
	Fe(Ⅲ)	32.4	—	16
Linear Range (μmol L^{-1})	$KBrO_3$	10-4264	1-932	10-5010
	KNO_2	100-8000	10-8000	100-8000
	Cr(VI)	1—	—	1—
	Fe(Ⅲ)	1—	—	1—
Sensitivity (μAcm^{-2} mM^{-1})	$KBrO_3$	6.91×10^{-4}	8×10^{-3}	2×10^{-3}
	KNO_2	1.367×10^{-4}	2×10^{-3}	2.4×10^{-4}
	Cr(VI)	1.1×10^{-1}	—	6.8×10^{-2}
	Fe(Ⅲ)	3.2×10^{-2}	—	3×10^{-3}

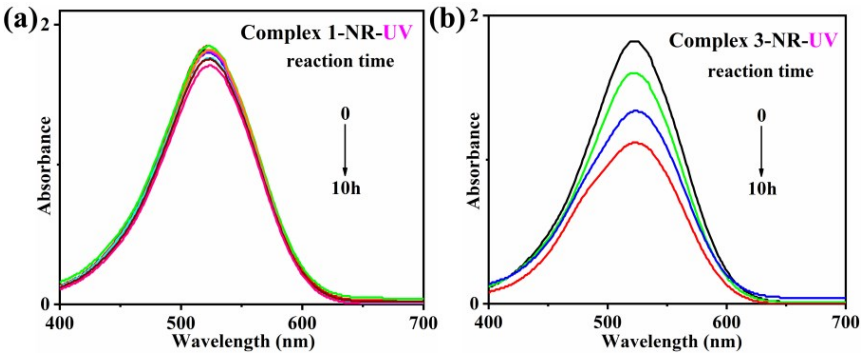

Fig. S7 Photocatalytic reaction of NR solutions in the presence of complexes **1** and **3** under UV irradiation.

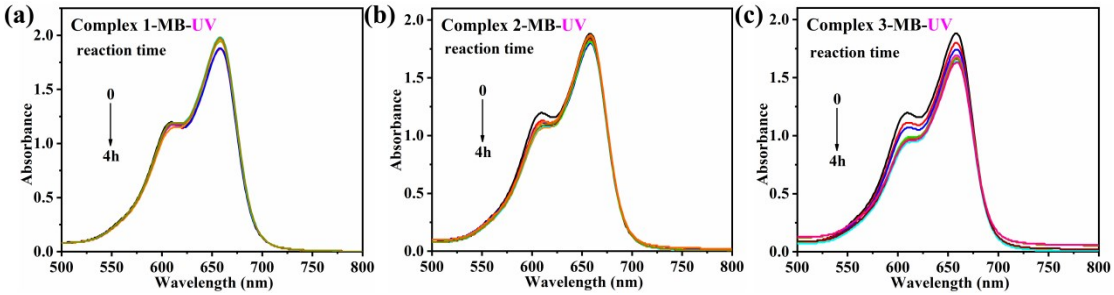

Fig. S8 Photocatalytic reaction of MB solutions in the presence of complexes **1-3** under UV irradiation.

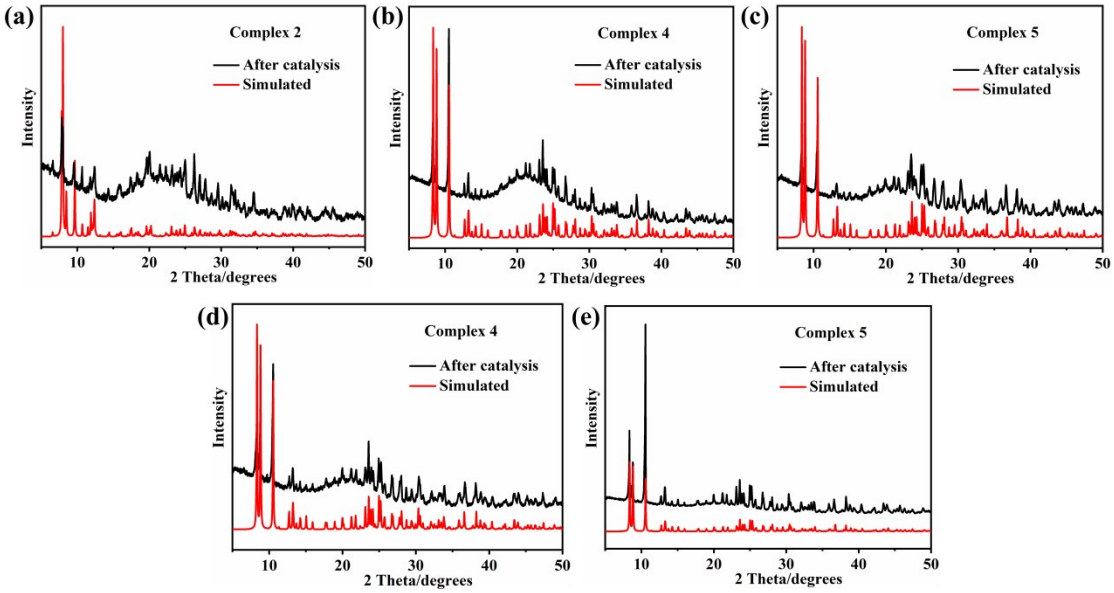

Fig. S9 (a-c) PXRD patterns of complexes **2**, **4** and **5** on NR after catalysis. (d-e) PXRD patterns of complexes **4** and **5** on MB after catalysis.