Supporting Information

Polymolybdate-directed Two Zn(II) Complexes Tuned by a New Bispyridine-bis-amide Ligand with Diphenylketone Spacer for Efficient Ampere Sensing and Dye Adsorption

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Materials and methods

(NH₄)₆[TeMo₆O₂₄]·7H₂O and Na₃[CrMo₆(OH)₆O₁₈]·8H₂O were prepared according to the literatures.^{1,2} The synthetic route of ligand L was similar to that of the reported amide-based organic ligands.³ The chemicals and solvents used in the experiments were purchased from commercial sources and used directly without further processing. The FT-IR spectroscopy recorded on Varian 640 IR spectrometer was used to further prove the crystal composition. PXRD data was recorded on D/teX Ultra diffractometer. All electrochemical tests were performed using CHI760 work station. A traditional threeelectrode system was used for testing, which includes carbon paste electrode (working electrode) made of complexes**1–2**, Ag/AgCl electrode (reference electrode) and Pt wire electrode (counter electrode).The UV-Vis absorption spectra of dye adsorption were collected on an SP-1901 UV-Vis spectrophotometer.

Synthesis of ligand L

Isonicotinic acid (4.92 g, 0.04 mmol) and 4,4-diaminobenzophenone (3.96 g, 0.02 mmol) were mixed into a 250 mL three-necked flask containing pyridine (60mL). Triphenyl phosphate (12.3 g, 0.04 mol) was slowly added after stirring for 30 minutes, and the mixture was refluxed for 10 hours. After cooling to room temperature, a white precipitate was obtained. The solid was filtered and washed with ethanol.

X-ray crystallography

A Bruker SMART APEXII system with Mo K α radiation ($\lambda = 0.71073$ Å) was used to collect and process crystallographic data. Solved by direct method, and the crystal

structure of complexes 1-2 were obtained by full-matrix least squares method based on F^2 in Olex2 software.⁴

 Table S1 Selected bond distances (Å) and angles (°) for complexes 1–2

Complex 1						
Zn(1)-O(1)	1.985(2)	O(1)-Zn(1)-N(4)#3	92.61(9)			
Zn(1)-O(6)#1	1.986(2)	O(6)#1-Zn(1)-O(2)#2	113.29(10)			
Zn(1)-O(2)#2	1.998(2)	O(6)#1-Zn(1)-N(1)	89.36(9)			
Zn(1)-N(1)	2.172(2)	O(6)#1-Zn(1)-N(4)#3	89.20(10)			
Zn(1)-N(4)#3	2.154(2)	O(2)#2-Zn(1)-N(1)	87.75(10)			
O(1)-Zn(1)-O(6)#1	124.38(10)	O(2)#2-Zn(1)-N(4)#3	91.27(10)			
O(1)-Zn(1)-O(2)#2	122.22(9)	N(4)#3-Zn(1)-N(1)	177.79(10)			
O(1)-Zn(1)-N(1)	89.58(9)					
Symmetry codes for 1:	#1 x, -y+1/2, z-1	/2 #2 -x+2, y+1/2, -z-1/2	#3 x+1, -y+1/2, z-			

3/2

Complex 2							
Zn(1)-O(1)	2.156(4)	O(1W)#1-Zn(1)-O(1W)	180				
Zn(1)-O(1)#1	2.156(4)	O(1W)-Zn(1)-N(6)#1	92.2(2)				
Zn(1)-O(1W)#1	2.130(6)	O(1W)-Zn(1)-N(6)	87.8(2)				
Zn(1)-O(1W)	2.130(6)	O(1W)#1-Zn(1)-N(6)#1	87.8(2)				
Zn(1)-N(6)	2.163(5)	O(1W)#1-Zn(1)-N(6)	92.2(2)				
Zn(1)-N(6)#1	2.163(5)	N(6)#1-Zn(1)-N(6)	180				
Zn(2)-O(2)	2.135(4)	O(2)-Zn(2)-O(2)#2	180				
Zn(2)-O(2)#2	2.135(4)	O(2W)#2-Zn(2)-O(2)	87.38(19)				
Zn(2)-O(2W)#2	2.038(5)	O(2W)-Zn(2)-O(2)#2	87.38(19)				
Zn(2)-O(2W)	2.038(5)	O(2W)#2-Zn(2)-O(2)#2	92.62(19)				
Zn(2)-O(3W)	2.117(6)	O(2W)-Zn(2)-O(2)	92.61(19)				
Zn(2)-O(3W)#2	2.117(6)	O(2W)#2-Zn(2)-O(2W)	180				
O(1)#1-Zn(1)-O(1)	180	O(2W)-Zn(2)-O(3W)	89.3(3)				
O(1)#1-Zn(1)-N(6)	92.03(18)	O(2W)#2-Zn(2)-O(3W)#2	89.3(3)				
O(1)-Zn(1)-N(6)	87.97(18)	O(2W)#2-Zn(2)-O(3W)	90.7(3)				
O(1)-Zn(1)-N(6)#1	92.03(18)	O(2W)-Zn(2)-O(3W)#2	90.7(3)				
O(1)#1-Zn(1)-N(6)#1	87.97(18)	O(3W)#2-Zn(2)-O(2)#2	92.8(2)				
O(1W)#1-Zn(1)-O(1)	92.15(17)	O(3W)-Zn(2)-O(2)	92.8(2)				
O(1W)#1-Zn(1)-O(1)#1	87.85(17)	O(3W)#2-Zn(2)-O(2)	87.2(2)				
O(1W)-Zn(1)-O(1)#1	92.15(17)	O(3W)-Zn(2)-O(2)#2	87.2(2)				
O(1W)-Zn(1)-O(1)	87.85(17)	O(3W)#2-Zn(2)-O(3W)	180.0(2)				

Symmetry codes for **2**: #1 -x, -y+1, -z+1 #2 -x+1, -y+1, -z+1

Complex	D–H···A	D–H / Å	H…A / Å	D…A / Å	D–H···A / °			
2	O2W−H2WB…O1W	0.85	1.98	2.805	165			
	N3-H3…O19	0.86	2.07	2.869	161			



Fig. S1. (a) 1D chain structure of complex 1 along different development directions: (a) c-axis and (b) b-axis.



Fig. S2. The PXRD patterns of complexes 1–2.



Fig. S4. Cyclic voltammetry curves of (a) 1–CPE (b) 2–CPE in different electrolyte solutions (scan rate: $60 \text{ mV} \cdot \text{s}^{-1}$).

600

-200

200 E / mV 400

600

Ö

-200

200 E / mV

0

400



Fig. S5. The best potential of amperometric detection of (a-b) Cr(VI) ions and (c-d) AA for 1–2–CPEs.



Fig. S6. The calibration curves between the current and concentration of (a-b) Cr(VI), (c-d) KBrO₃, (e-f) H₂O₂ and (g-h) AA which measured by 1–2–CPEs.



Fig. S7. The PXRD of 1–2–CPEs after working 10 h.



Fig. S8. The calibration curves between the current and concentration of Cr(VI) which measured by 1-2-CPEs in the real water sample.



Fig. S9. The absorption peaks of complex 1 for cationic dye CV and MB at dark.



Fig. S10. The absorption peaks of complex 2 for cationic dye CV at dark during adsorption and desorption. Inset is the color change of complex 2 after adsorption and desorption of cationic dye CV.



Fig. S11. The absorption peaks of complexes 1–2 for anionic dye MO at dark.

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