Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry

Two Unusual 3D Honeycomb Network Based on Wells-Dawson Arsenomolybdates with d^{10} Transition-Metal-Pyrazole Connectors

Bo-Wen Cong,[a] Zhan-Hua Su,* [a] Bao-Yi Yu,[c] Wen-Qi Zhao, [a] Xiu-Juan Ma,[a] and Zhi-Feng Zhao, *[b]

[a]*Key Laboratory of Synthesis of Functional Materials and Green Catalysis, Colleges of Heilongjiang Province, Harbin Normal University, Harbin 150025, China*

[b]*College of Material Science and Engineering, University of Science and Technology Heilongjiang, Harbin 150022, China*

[c]*Beijing University of Agriculture, 102206, China*

Table S1 Selected bond lengths (Å) and bond angles (°) of compounds **1** and **2**

Compound **1**					
Mo(1)-O(1)	1.686(5)	Mo(1)-O(3)	1.822(4)	Mo(1)-O(4)	1.923(4)
Mo(1)-O(2)#1	1.943(5)	Mo(1)-O(2)	2.038(5)	Mo(1)-O(5)	2.360(4)
Mo(2)-O(6)	1.653(5)	Mo(2)-O(9)	1.787(9)	Mo(2)-O(11)#1	1.810(9)
Mo(2)-O(4)	1.953(4)	Mo(2)-O(7)	1.967(5)	Mo(2)-O(11A)#1	2.007(9)
Mo(2)-O(9A)	2.021(9)	Mo(2)-O(10A)#1	2.317(8)	Mo(2)-O(10)	2.367(8)
Mo(3)-O(8)	1.668(5)	Mo(3)-O(11)	1.795(8)	Mo(3)-O(9)	1.797(9)
Mo(3)-O(7)#2	1.835(5)	Mo(3)-O(9A)	2.028(9)	Mo(3)-O(11A)	2.057(9)
Mo(3)-O(3)#3	2.083(4)	Mo(3)-O(10A)	2.290(8)	Mo(3)-O(10)	2.325(8)
As(1)-O(10A)#3	1.682(9)	As(1)-O(10A)#1	1.682(9)	As(1)-O(10A)	1.682(9)
As(1)-O(10)#3	1.706(8)	As(1)-O(10)#1	1.706(8)	As(1)-O(10)	1.706(8)
As(1)-O(5)	1.722(7)	O(2)-Mo(1)#3	1.943(5)	O(3)-Mo(3)#1	2.083(4)
O(5)-Mo(1)#3	2.360(4)	O(5)-Mo(1)#1	2.360(4)	O(7)-Mo(3)#4	1.835(5)
O(10A)-Mo(2)#3	2.317(7)	O(11)-Mo(2)#3	1.810(9)	O(11A)-Mo(2)#3	2.007(9)
Cu(1)-N(1)#5	1.879(7)	Cu(1)-N(1)	1.879(7)	Cu(1)-O(9A)	2.598(1)
Cu(2)-O(8)	2.612(1)				
O(1)-Mo(1)-O(3)	104.0(2)	O(1)-Mo(1)-O(4)	102.9(2)	O(3)-Mo(1)-O(4)	89.64(19)
O(1)-Mo(1)-O(2)#1	99.3(2)	O(3)-Mo(1)-O(2)#1	92.6(2)	O(4)-Mo(1)-O(2)#1	156.44(19)
O(1)-Mo(1)-O(2)	97.5(2)	O(3)-Mo(1)-O(2)	158.50(19)	O(4)-Mo(1)-O(2)	84.55(18)
O(2)#1-Mo(1)-O(2)	84.8(3)	O(1)-Mo(1)-O(5)	167.1(2)	O(3)-Mo(1)-O(5)	87.12(18)
O(4)-Mo(1)-O(5)	83.47(16)	O(2)#1-Mo(1)-O(5)	73.24(16)	O(2)-Mo(1)-O(5)	71.68(16)
O(6)-Mo(2)-O(9)	112.3(4)	O(6)-Mo(2)-O(11)#1	116.2(4)	O(9)-Mo(2)-O(11)#1	130.7(5)
O(6)-Mo(2)-O(4)	98.5(2)	O(9)-Mo(2)-O(4)	89.5(3)	O(11)#1-Mo(2)-O(4)	91.3(3)
O(6)-Mo(2)-O(7)	95.9(2)	O(9)-Mo(2)-O(7)	87.5(3)	O(11)#1-Mo(2)-O(7)	79.9(3)
O(4)-Mo(2)-O(7)	165.33(19)	O(6)-Mo(2)-O(11A)#1	91.3(3)	O(9)-Mo(2)-O(11A)#1	155.9(4)
O(4)-Mo(2)-O(11A)#1	82.2(3)	O(7)-Mo(2)-O(11A)#1	94.8(3)	O(6)-Mo(2)-O(9A)	89.3(3)

O(11)#1-Mo(2)-O(9A)	153.7(4)	O(4)-Mo(2)-O(9A)	90.7(3)	O(11A)#1-Mo(2)-O(9A)	172.9(3)
O(6)-Mo(2)-O(10A)#1	161.6(3)	O(9A)-Mo(2)-O(10A)#1	109.0(3)	O(6)-Mo(2)-O(10)	157.4(3)
O(11)#1-Mo(2)-O(10)	85.6(4)	O(11A)#1-Mo(2)-O(10)	111.3(3)	O(8)-Mo(3)-O(11)	114.8(4)
O(11)-Mo(3)-O(9)	132.2(4)	O(8)-Mo(3)-O(7)#2	99.8(2)	O(11)-Mo(3)-O(7)#2	84.8(3)
O(11)-Mo(3)-O(9A)	155.0(4)	O(9)-Mo(3)-O(11A)	152.8(4)	O(7)#2-Mo(3)-O(11A)	99.0(3)
O(9A)-Mo(3)-O(11A)	163.9(3)	O(8)-Mo(3)-O(3)#3	92.6(2)	O(7)#2-Mo(3)-O(3)#3	167.1(2)
O(8)-Mo(3)-O(10A)	158.7(3)	O(9A)-Mo(3)-O(10A)	108.6(3)	O(8)-Mo(3)-O(10)	158.6(3)
O(10)#3-As(1)-O(10)#1	108.9(3)	As(1)-O(5)-Mo(1)#3	122.17(14)	As(1)-O(10)-Mo(3)	122.8(4)
Mo(3)-O(11)-Mo(2)#3	155.1(5)	Mo(2)#3-O(11A)-Mo(3)	120.0(4)	N(1)#5-Cu(1)-N(1)	179.8(5)

Symmetry transformations used to generate equivalent atoms: #1 -y+1,x-y+1,z; #2 y-1/3,-x+y+1/3,-z+4/3; #3 -x+y,-x+1,z; #4 x-y+2/3,x+1/3,-z+4/3; #5 -x+4/3,-x+y+2/3,-z+7/6

Compound **2**					
Ag(1)-N(1)#1	2.112(6)	Ag(1)-N(1)	2.112(6)	Ag(2)-N(3)	2.108(6)
Ag(2)-N(3)#2	2.108(6)	Mo(1)-O(10)	1.652(3)	Mo(1)-O(9)	1.786(7)
Mo(1)-O(3)	1.883(3)	Mo(1)-O(8)	1.995(6)	Mo(1)-O(6)#3	2.037(4)
Mo(1)-O(7)	2.318(5)	Mo(2)-O(2)	1.685(4)	Mo(2)-O(4)	1.799(3)
Mo(2)-O(1)	1.898(3)	Mo(2)-O(3)	1.989(3)	Mo(2)-O(1)#4	2.046(3)
Mo(2)-O(11)	2.360(3)	Mo(3)-O(5)	1.666(4)	Mo(3)-O(6)	1.796(4)
Mo(3)-O(9)#5	1.798(7)	Mo(3)-O(8)	2.063(6)	Mo(3)-O(4)	2.127(3)
Mo(3)-O(7)	2.289(5)	As(1)-O(7)	1.644(5)	As(1)-O(11)	1.715(5)
O(1)-Mo(2)#5	2.046(3)	O(6)-Mo(1)#6	2.037(4)	O(11)-Mo(2)#4	2.360(3)
O(11)-Mo(2)#5	2.360(3)	O(9)-Mo(3)#4	1.797(6)	Ag(1)-O(9A)	2.660
Ag(2)-O(5)	2.708				
N(1)#1-Ag(1)-N(1)	176.6(3)	N(3)-Ag(2)-N(3)#2	174.1(4)	O(10)-Mo(1)-O(9)	111.7(3)
O(10)-Mo(1)-O(3)	100.87(17)	O(9)-Mo(1)-O(3)	90.8(2)	O(10)-Mo(1)-O(8)	92.0(2)
O(9)-Mo(1)-O(8)	156.3(3)	O(3)-Mo(1)-O(8)	83.68(19)	O(10)-Mo(1)-O(6)#3	93.70(17)
O(9)-Mo(1)-O(6)#3	86.0(2)	O(3)-Mo(1)-O(6)#3	165.24(14)	O(8)-Mo(1)-O(6)#3	93.6(2)
O(10)-Mo(1)-O(7)	162.1(2)	O(9)-Mo(1)-O(7)	86.0(3)	O(6)#3-Mo(1)-O(7)	85.16(17)
O(2)-Mo(2)-O(4)	104.77(17)	O(2)-Mo(2)-O(1)	100.93(17)	O(4)-Mo(2)-O(1)	95.52(15)
O(2)-Mo(2)-O(3)	101.32(17)	O(4)-Mo(2)-O(3)	88.36(14)	O(1)-Mo(2)-O(3)	155.62(14)
O(2)-Mo(2)-O(1)#4	96.64(16)	O(4)-Mo(2)-O(1)#4	157.86(14)	O(1)-Mo(2)-O(1)#4	85.7(2)
O(3)-Mo(2)-O(1)#4	81.91(13)	O(2)-Mo(2)-O(11)	167.24(17)	O(4)-Mo(2)-O(11)	87.50(14)
O(1)-Mo(2)-O(11)	73.98(12)	O(3)-Mo(2)-O(11)	82.17(12)	O(1)#4-Mo(2)-O(11)	71.55(12)
O(5)-Mo(3)-O(6)	100.71(18)	O(5)-Mo(3)-O(9)#5	111.6(3)	O(6)-Mo(3)-O(9)#5	95.6(3)
O(5)-Mo(3)-O(8)	88.4(2)	O(6)-Mo(3)-O(8)	101.4(2)	O(9)#5-Mo(3)-O(8)	150.9(3)
O(5)-Mo(3)-O(4)	90.96(16)	O(6)-Mo(3)-O(4)	167.80(14)	O(9)#5-Mo(3)-O(4)	83.2(2)
O(8)-Mo(3)-O(4)	75.15(18)	O(5)-Mo(3)-O(7)	156.50(19)v	O(6)-Mo(3)-O(7)	92.38(18)
O(9)#5-Mo(3)-O(7)	86.1(3)	O(8)-Mo(3)-O(7)v	69.8(2)	O(4)-Mo(3)-O(7)	75.42(16)
O(7)#4-As(1)-O(7)	114.68(14)	O(7)#4-As(1)-O(11)	103.56(19)	As(1)-O(11)-Mo(2)#4	122.86(11)

Symmetry transformations used to generate equivalent atoms: #1 x-y+2/3,-y+4/3,-z+5/6; #2 y+2/3,x-2/3,-z+5/6; #3 x-y+1/3,x-1/3,-z+2/3; #4 -y+1,x-y,z; #5 -x+y+1,-x+1,z; #6 y+1/3,-x+y+2/3,-z+2/3

Table S2 Hydrogen bonds information for compounds **1** and **2**

Compound **1**

D-H…A	d(D…H) Å	d(H…A) Å	d(D…A) Å	∠(DHA)°
N(2) --H(2) ..O(4)	0.86	2.24	2.982(11)	144
N(2) --H(2) ..O(3)#1	0.86	2.54	3.198(10)	134
N(4) --H(4) ..O(8)	0.86	2.42	3.019(12)	127
C(1) --H(1) ..O(9A)#2	0.93	2.44	3.023(14)	120
C(1) --H(1) ..O(11)#3	0.93	2.58	3.318(16)	136
C(5) --H(5) ..O(6)#4	0.93	2.44	3.279(18)	150

Symmetry transformations used to generate equivalent atoms: #1 -x+y,1-x,z; #2 4/3-x,2/3-x+y,7/6-z; #3 2/3-x+y,1/3+y,-1/6+z; #4 1+x-y,x,1-z

Compound **2**

D-H…A	d(D…H) Å	d(H…A) Å	d(D…A) Å	∠(DHA)°
N(4) --H(4)..O(4)	0.86	2.59	3.381(10)	153
N(4) --H(4)..O(5)	0.86	2.48	3.105(8)	130
C(4) --H(4A)..O(2)	0.93	2.56	3.245(14)	130
C(5) --H(5)..O(10)#1	0.93	2.50	3.245(13)	137

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

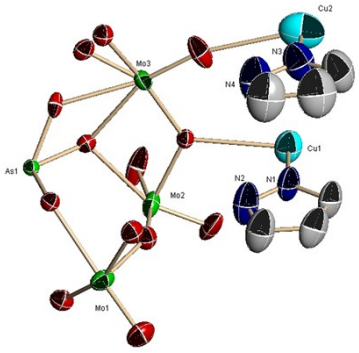


Fig. S1 Asymmetric unit of compound **1** (all of the hydrogen atoms are ommitted for clarity)

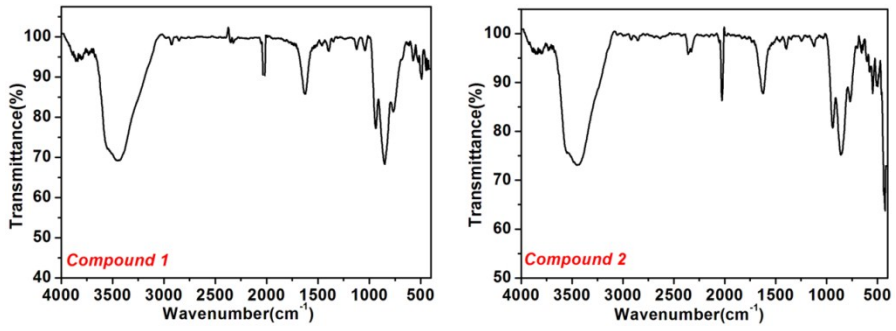


Fig. S2 IR spectra of compounds **1** and **2**

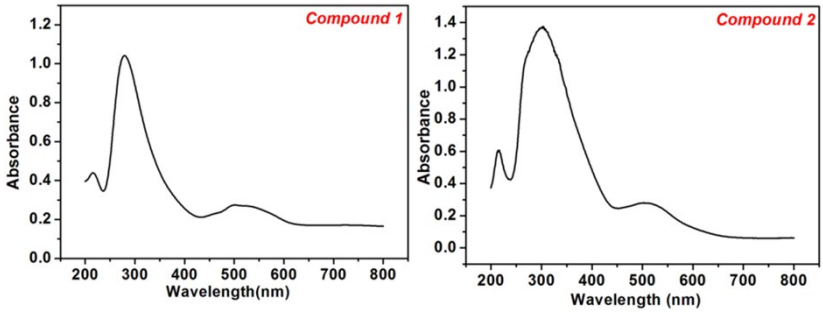
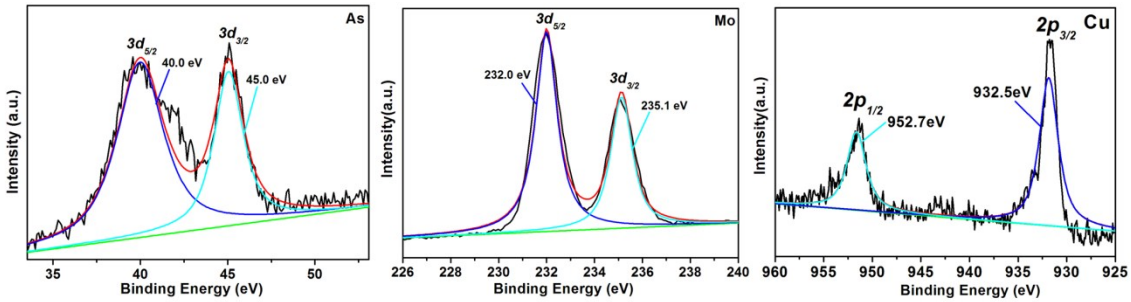


Fig. S3 The UV-vis spectra of compounds **1** and **2** in solid state at room temperature

Compound 1



Compound 2

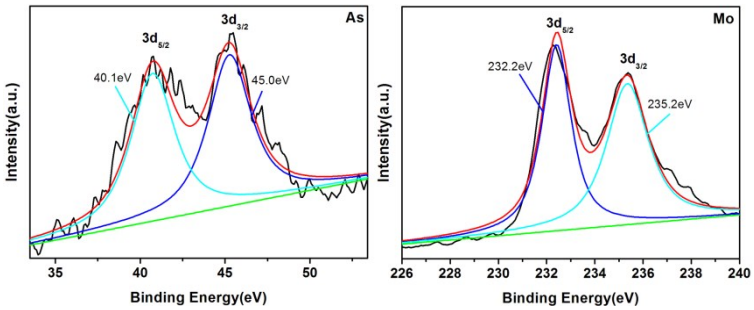


Fig. S4 The XPS spectra of compounds **1** and **2**

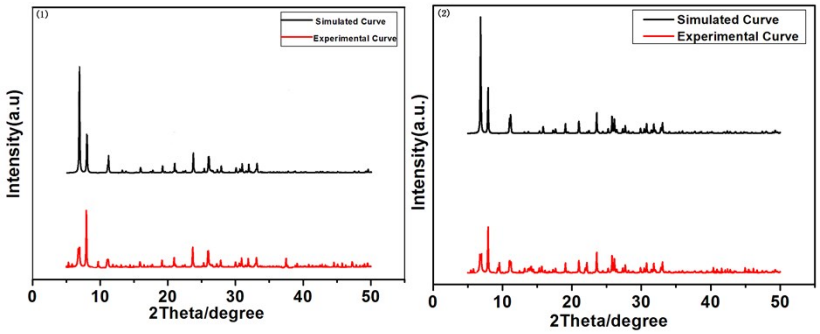


Fig. S5 The PXRD contrast curves of compounds **1** and **2**

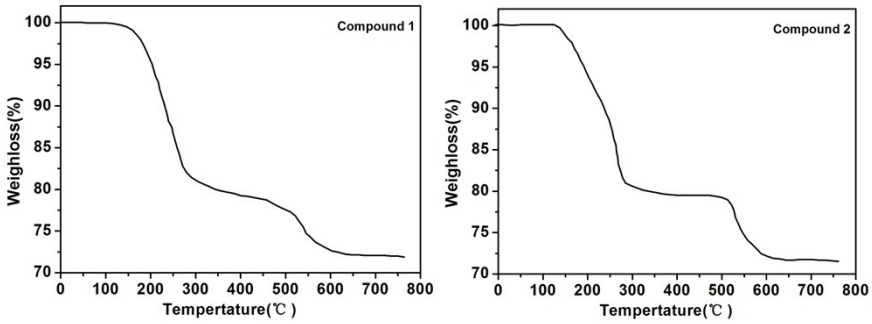


Fig. S6 TG curves of compounds **1** and **2**

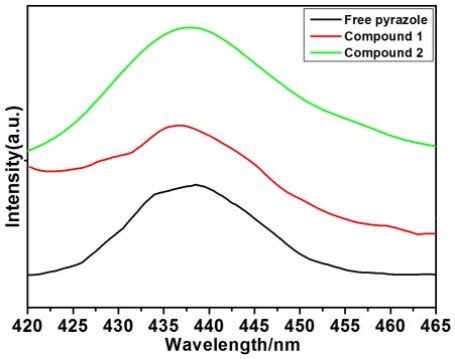


Fig. S7 Fluorescence spectra of compounds **1** and **2** in the solid state at room temperature

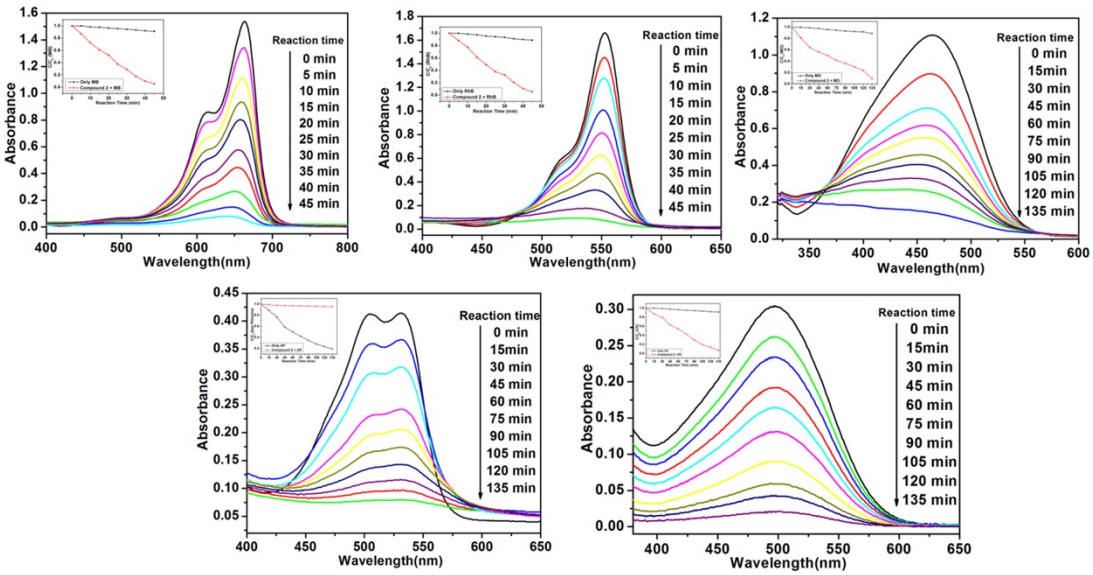


Fig. S8 UV-vis absorption spectra of the MB, RhB, MO, AP, and CR solutions during the decomposition reaction under UV irrdiation in the presence of compound **2 (**insets) Absorption spectra of the five dyes solution during the decomposition reaction under UV irradiation in the presence of compound **2**

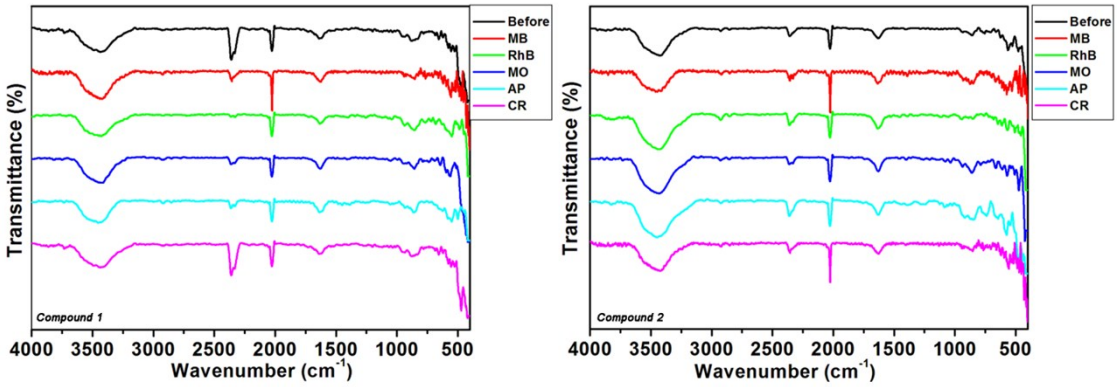


Fig. S9 The IR spectra of catalyst **1** and **2** before and after cycle reaction

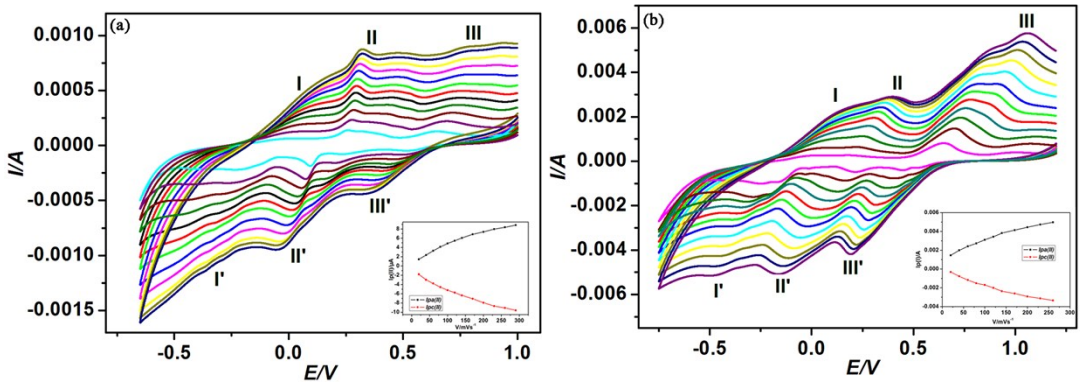


Fig. S10 Cyclic voltammograms of (a) **1-CPE** and (b) **2-CPE** rates (from inner to outer: 20, 40, 60, 80, 100, 120, 140, 170, 200, 230, 260, 290 mV s^{-1}). Potentials vs. SCE. (Insert plots: The dependence of anodic peak II current on scan rates.)