Electronic Supplementary Information (ESI)

A Series of Isopolymolybdate-viologen Hybrids with Photo-, Thermo- and Electro-chromic Properties

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Materials and General Methods

All reagents and solvents were purchased from commercial sources except 1,3–bcbpy·2Cl, 1,4–bcbpy·2Cl and 1,1–pmbby·2Cl, which were synthesized based on literature reports.[1-3] So there was no further purification before their use. The FT-IR spectra were taken on a Varian FT–IR 640 spectrometer (KBr pellets) in the range of 400–4000 cm^{-1}. Powder X–ray diffraction (PXRD) patterns were recorded on an Ultima IV with D/teX Ultra diffractometer at 40 kV, 40 mA with Cu Kα (λ = 1.5406 Å) radiation in the 2θ range of 5–50°. UV–Vis absorption spectra were obtained using a UV–1801 ultra violet spectrophotometer.

Preparation of compounds 1–4

Synthesis of (1,3–bcbpy)$_2$·(δ–Mo_8O_{26}) (1)

$Cd(NO_3)_2·4H_2O$ (0.1 g, 0.4 mmol), $(NH_4)_6Mo_7O_{24}·4H_2O$ (0.1 g, 0.08 mmol) and 1,3–bcbpy·2Cl (0.02 g, 0.01 mmol) were dissolved in 20 ml distilled water at room temperature. The suspension was stirred at room temperature for 1 h. Then the pH was adjusted to about 3.97 with 1.0 mol·L^{-1} HNO_3 and 1.0 mol·L^{-1} NaOH, and the suspension was sealed in a Teflon–lined autoclave (25 ml) and maintained at 150 ℃ for 7 d. After cooling to room temperature at the rate of 10 ℃·h^{-1}, the colorless block

crystal of **1** was collected and washed with distilled water (yield 38% based on Mo). Anal. Calcd for **1** $C_{52}H_{44}Mo_8N_4O_{34}$ (2036.43): C 30.64, H 2.16, N 2.75%. Found: C 30.62, H 2.13, N 2.74%.

Synthesis of {Co(1,4–bcbpy)$_2$(H$_2$O)$_2$[H$_2$(β–Mo$_8$O$_{26}$)]}·2H$_2$O·2CH$_2$O (2)

$CoCl_2·6H_2O$ (0.1 g, 0.73 mmol), MoO_3 (0.1 g, 0.69 mmol) and 1,4–bcbpy·2Cl (0.05 g, 0.09 mmol) were added to a mixture of 3 mL DMF and 5 mL distilled water, and stirred continuously for 60 min. The mixture was transferred to a 10 mL glass bottle and heated at 90°C for 4 d. The temperature was reduced to room temperature with a rate of 5 °C per hour. The product was washed with deionized water and dried. The light pink block crystals of **2** were obtained (yield 34% based on Mo). Anal. Calcd. for $C_{54}H_{54}CoMo_8N_4O_{40}$ (2225.44): C 29.12, H 2.43, N 2.52% Found: C 29.11, H 2.42, N 2.50%.

Synthesis of (1,4–bcbpy)$_2$·(δ–Mo$_8$O$_{26}$) ·2H$_2$O (3)

$NiSO_4·2H_2O$ (0.1 g, 0.4 mmol), $(NH_4)_6Mo_7O_{24}·4H_2O$ (0.1 g, 0.08 mmol) and 1,4–bcbpy·2Cl (0.02 g, 0.01 mmol) were dissolved in 20 ml distilled water at room temperature. The suspension was stirred at room temperature for 1 h. Then the pH was adjusted to about 3.84 with 1.0 mol·L^{-1} HNO_3 and 1.0 mol·L^{-1} NaOH, and the suspension was sealed in a Teflon–lined autoclave (25 ml) and maintained at 150 ℃ for 7 d. After cooling to room temperature at the rate of 10 ℃·h^{-1}, the light yellow block crystal of **3** was collected and washed with distilled water (yield 37% based on Mo). Anal. Calcd for **3** $C_{52}H_{48}Mo_8N_4O_{36}$ (2072.46): C 30.11, H 2.32, N 2.70%. Found: C 30.10, H 2.31, N 2.67%.

Synthesis of {Cu(1,1–pmbby)$_2$(H$_2$O)[H$_2$(β–Mo$_8$O$_{26}$)$_2$]}·5H$_2$O·C$_2$H$_7$N (4)

$CuCl_2·2H_2O$ (0.1 g, 0.73 mmol), MoO_3 (0.1 g, 0.69 mmol) and 1,1–pmbby·2Cl (0.05 g, 0.09 mmol) were added to a mixture of 3 mL DMF and 5 mL distilled water, and stirred continuously for 60 min. The mixture was transferred to a 10 mL glass bottle and heated at 90°C for 4 d. The temperature was reduced to room temperature with a rate of 5 °C per hour. The product was washed with deionized water and dried. The blue block crystals of **4** were obtained (yield 45% based on Mo). Anal. Calcd. for $C_{58}H_{69}CuMo_{16}N_9O_{58}$ (3418.78): C 20.36, H 2.02, N 3.69% Found: C 20.34, H 2.00, N

3.68%.

Photoelectrochemical measurement

The photocurrent measurements were recorded on a CHI660E Electrochemical Workstation with a three-electrode configuration that the platinum plate, Ag/AgCl electrode and catalyst modified electrode acted as the counter electrode, reference electrode and working electrode, respectively. A 0.2 M Na_2SO_4 solution was used as the electrolyte. A 300 W Xe lamp (CEL–HXF300–T3, Beijing Zhongjiao Jinyuan Technology Co., Ltd) was used as the light source.

The preparation of working electrode

Indium tin oxide (ITO) glass was ultrasonically washed with ethanol for 30 min, then rinsed with deionized water and dried for use. 10 mg of grinded crystals were added into 0.4 mL 0.5% Nafion solution with isopropanol. The suspension was ultrasonically mixed for 1 h, which dripped onto ITO glass with a coating of 10 × 10 mm^2. The prepared working electrode was dried at 60 °C for 3 h.

Preparation of 1/2/3/4–CPE

The compond **1**/**2**/**3**/**4** modified carbon paste electrode (**1**/**2**/**3**/**4**–CPE) were made as follows: a mixture of graphite powder (0.10 g) and compond **1** (0.01 g) was ground together by using an agate mortar for about 15 min. Then, while stirring, 0.1 mL of liquid paraffin was added to the resulting mixture. After that, the mixture was stuffed into a glass tube with an inner diameter of 1.5 mm. And then the surface of the glass tube was wiped with weighing paper. In the same manner, the **2**/**3**/**4**–CPE was made with compounds **2**, **3** and **4**.

Fabrication of electrochromic devices

To study the electrochromic properties of compounds **1**–**4**, the corresponding electrochromic devices were prepared. The following are the steps used for the fabrication of a rigid electrochromic device. Two ITO–glasses (2 × 3 cm) were used to create a slit-type rigid electrochromic device with a slit thickness (d) of ~50 mm. The electrochromic solution contained 0.01 M of compounds **1**–**4**, 0.01 M ferrocene,

and 0.1 M TBAP dissolved in PC. TBAP was used as electrolyte and ferrocene was the anode species in the electrochromic solution, which is an essential compound to compensate for charge neutrality in the faradaic reaction. Then, the electrochromic solution was injected into the device. Finally, the electrochromic devices for compounds **1**–**4** were successfully obtained (**1**/**2**/**3**/**4**–ECD).

X–ray crystallographic study

A Bruker SMART APEX II with Mo–Kα radiation (λ = 0.71073 Å) was used to collect X–Ray diffraction analyses data. All the structures were solved by direct methods and refined on F^2 by full-matrix least squares using the SHELXS-14 package.[4] The crystal data and structure refinement of compounds **1**–**4** are shown in Table S1. Selected bond lengths and angles of compounds **1**–**4** are summarized in Table S2. The CCDC numbers are 2224945, 2230421, 2224931 and 2224927 for **1**–**4** (Cambridge Crystallographic Data Center).

Table S1. Crystal data and structure refinements for compounds **1**–**4**.

Compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{52}H_{44}Mo_8N_4O_{34}$	$C_{54}H_{54}CoMo_8N_4O_{40}$	$C_{52}H_{48}Mo_8N_4O_{36}$	$C_{58}H_{69}CuMo_{16}N_9O_{58}$
Formula weight	2036.43	2225.44	2072.46	3418.78
Crystal system	Triclinic	Monoclinic	Monoclinic	Triclinic
Space group	P-1	C2/m	$P2_1/n$	P-1
a/Å	10.9560(6)	12.7429(4)	13.6738(4)	15.3467(3)
b/Å	11.1745(6)	20.7101(6)	11.8186(3)	16.5545(3)
c/Å	15.9449(11)	12.6924(7)	19.9517(6)	21.5569(4)
α/°	69.5270(10)	90	90	96.1750(10)
β/°	73.0910(10)	99.1440(10)	102.2930(10)	101.5210(10)
γ/°	63.6740(10)	90	90	110.1720(10)
Volume/Å^3	1617.57(17)	3307.0(2)	3150.37(15)	4943.61(16)
Z	1	2	2	2
D_c (g·cm^{-3})	2.091	2.173	2.185	2.204
μ/mm^{-1}	1.596	1.811	1.643	2.255

F(000)	992.0	2110.0	2024.0	3132.0
R_1[a] [I > 2σ(I)]	0.0332 0.0508	0.0294 0.0391	0.0430 0.0575	0.0497 0.0764
wR_2[b] (all data)	0.0668 0.0734	0.0666 0.0745	0.0984 0.1094	0.1154 0.1313
GOF on F^2	1.029	1.190	1.074	1.031

[a] $R^1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; [b] $wR^2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S3. TG results for compounds **2** and **4**.

Compound	**2**	**4**
cal. %	3.24	3.16
observed %	3.22	3.13

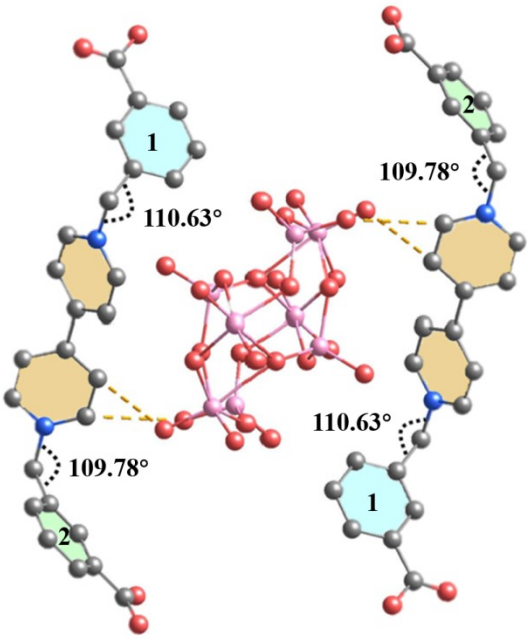

Fig. S1. The angles in the asymmetric unit of compound **1**.

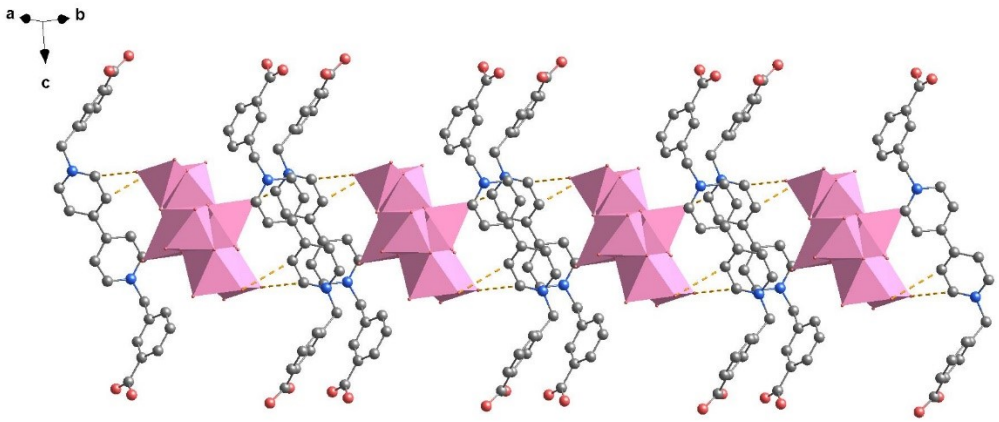

Fig. S2. The supramolecular 1D chain of compound **1**.

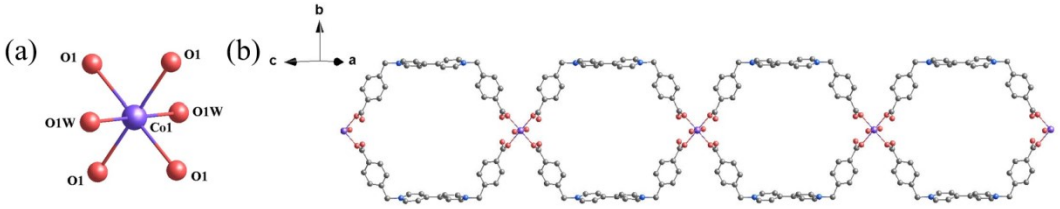

Fig. S3. (a) Coordination environment of metal Co1. (b) The metal-organic 1D chain of **2**.

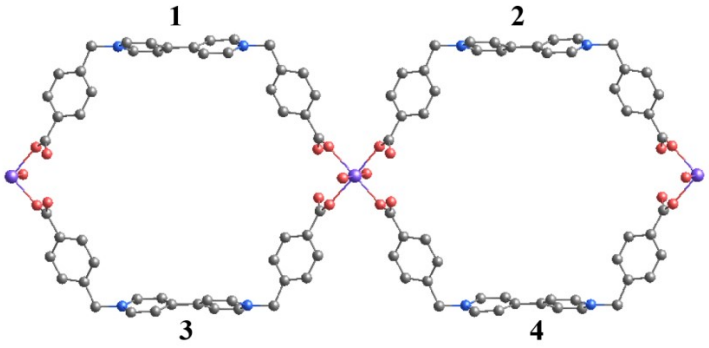

Fig. S4. Branches 1-4 in $[Co_3(1,4\text{-bcbpy})_4]^{6+}$.

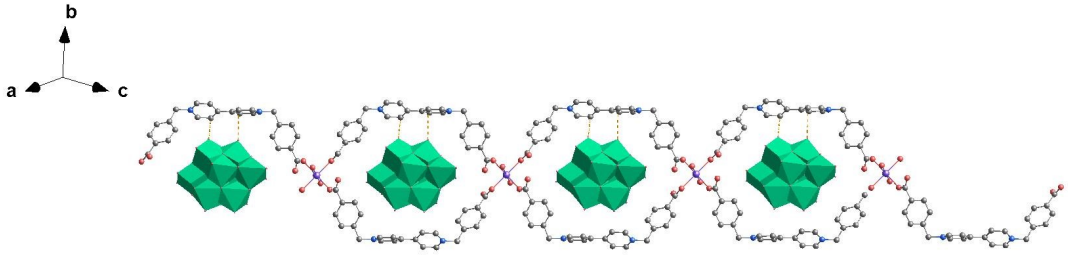

Fig. S5. The 1D chain of **2**.

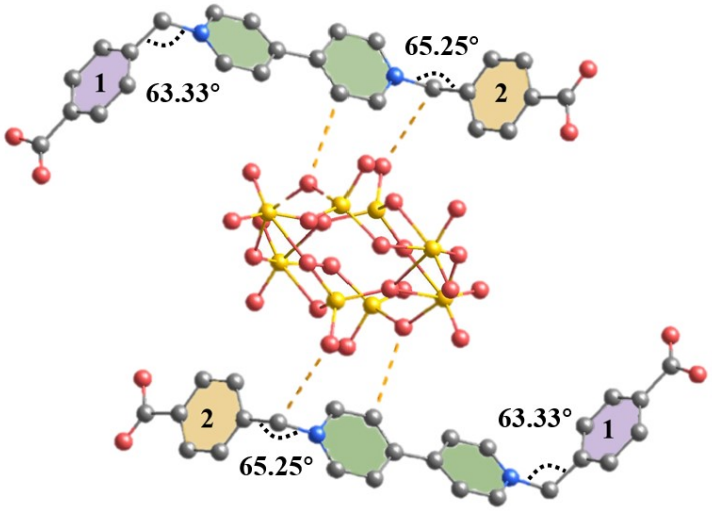

Fig. S6. The angles in the asymmetric unit of compound **3**.

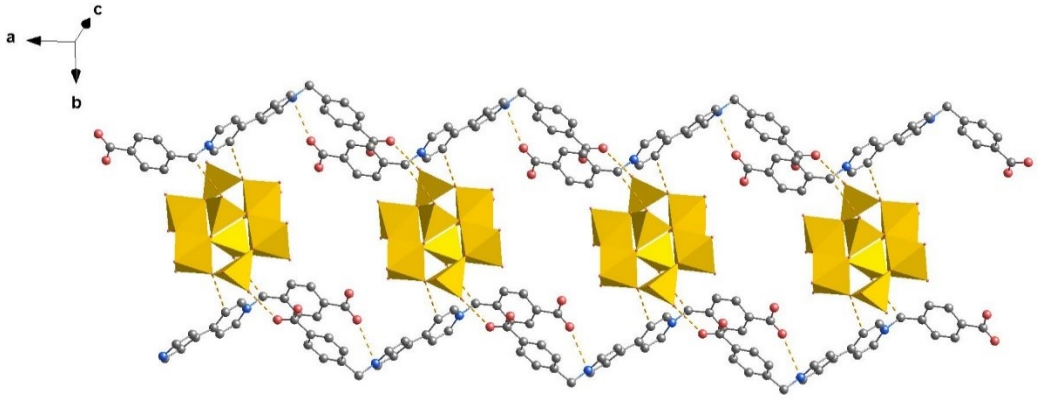

Fig. S7. The supramolecular 1D chain of compound **3**.

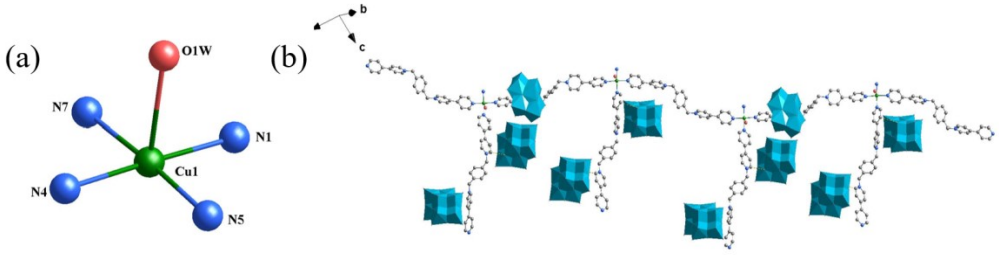

Fig. S8. (a) Coordination environment of metal Cu1. (b) The 1D chain of compound **4**.

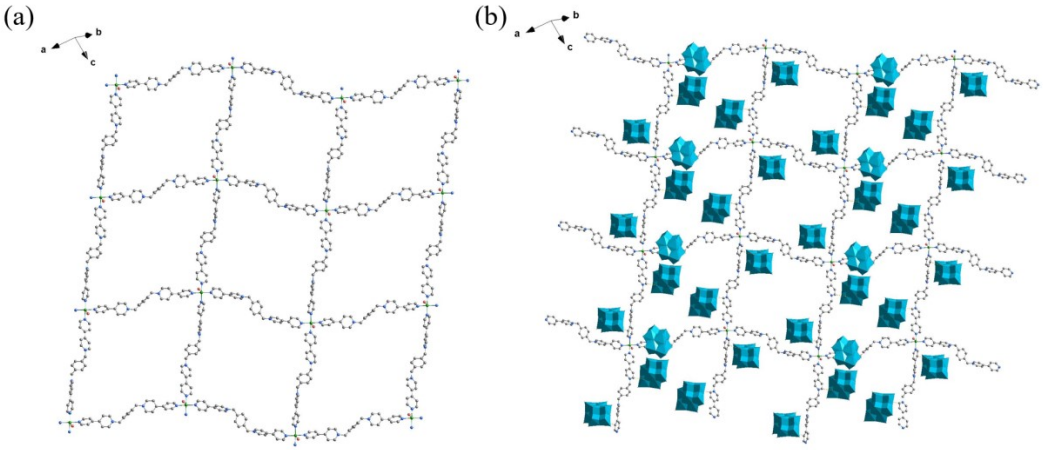

Fig. S9. (a)The metal-organic layer of compound **4**. (b) The 2D layer of **4**.

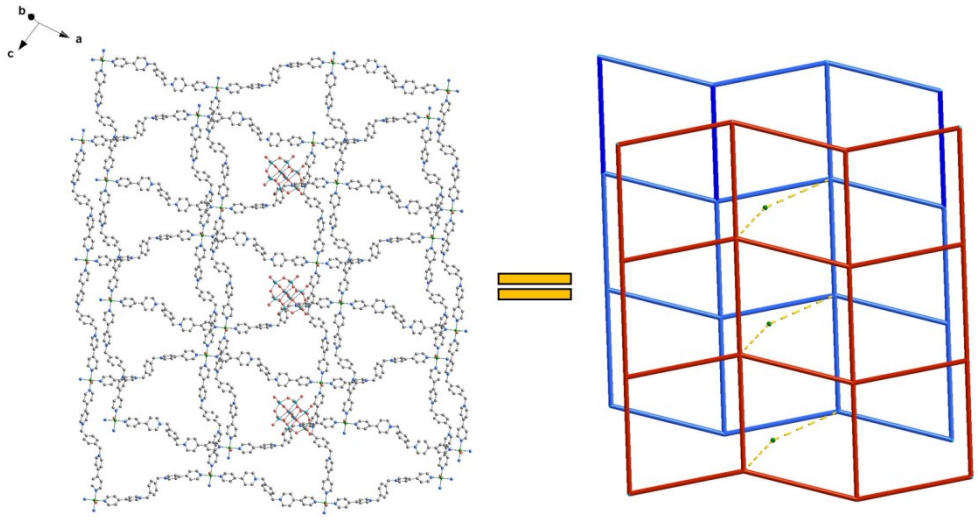

Fig. S10. The 3D supramolecular framework of compound **4**.

FT–IR Spectra and TG Analysis

The FT–IR spectra of compounds **1**–**4** was shown in Figure S11. The characteristic peaks at 914, 818, 726 and 655 cm^{-1} for **1**, 913, 819, 724 and 653 cm^{-1} for **3** are attributed to the δ–Mo_8 anion, and peaks at 914, 663 cm^{-1} for **2**, 912, 662 cm^{-1} for **4** are attributed to the β–Mo_8 anion.[5-6] The characteristic peaks in the region of 1766–1002 cm^{-1} for **1**, 1763–1005 cm^{-1} for **2**, 1765–1008 cm^{-1} for **3** and 1762–1009 cm^{-1} for **4**, are attributed to 1,3–bcbpy in **1**, 1,4–bcbpy in **2** and **3** and 1,1–pmbby in **4**, respectively.[7-9] What's more, we also analyzed the TG curves of compounds **2** and **4** (Figure S12). **2** and **4** have two main weightlessness processes. The mass loss in the first step below 300 ℃ is attributed to the loss of water molecules and free organic solvents, while the mass loss in the second step within the range of 400–800 ℃ is attributed to the loss of organic ligands. Within the range of 50–800 ℃, the total weight loss rate of **2** and **4** is consistent with the calculated value (Table S3).

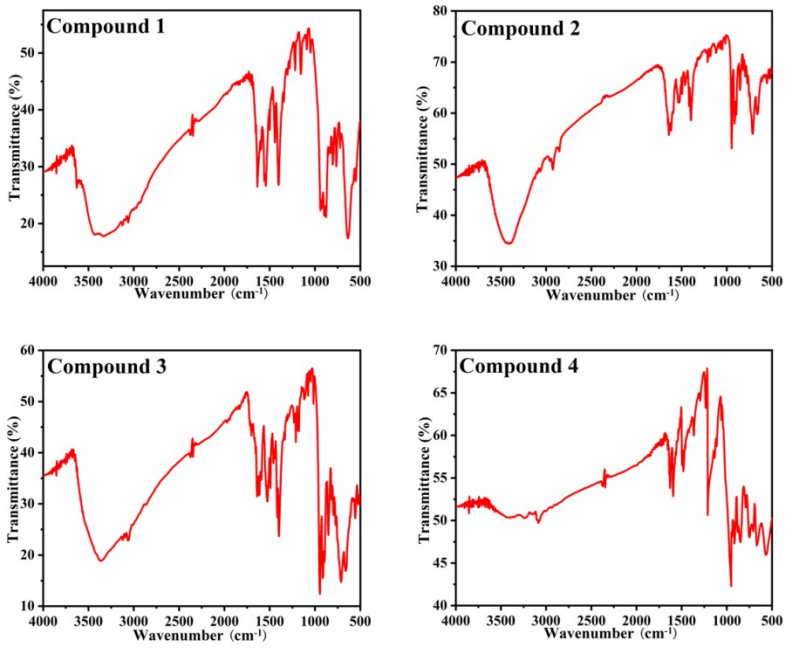

Fig. S11. The FT–IR spectra of compounds **1**–**4**.

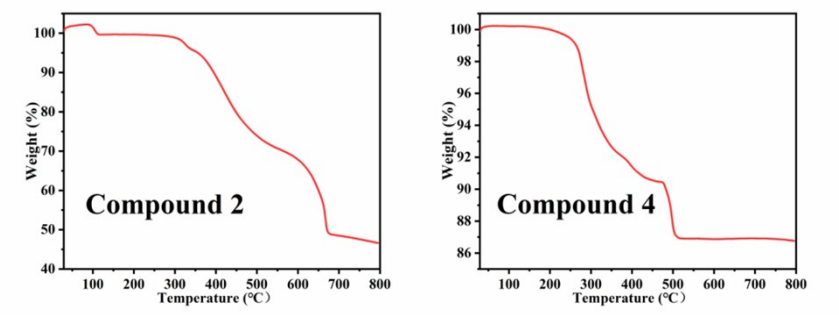

Fig. S12. The TG curves of compounds **2** and **4**.

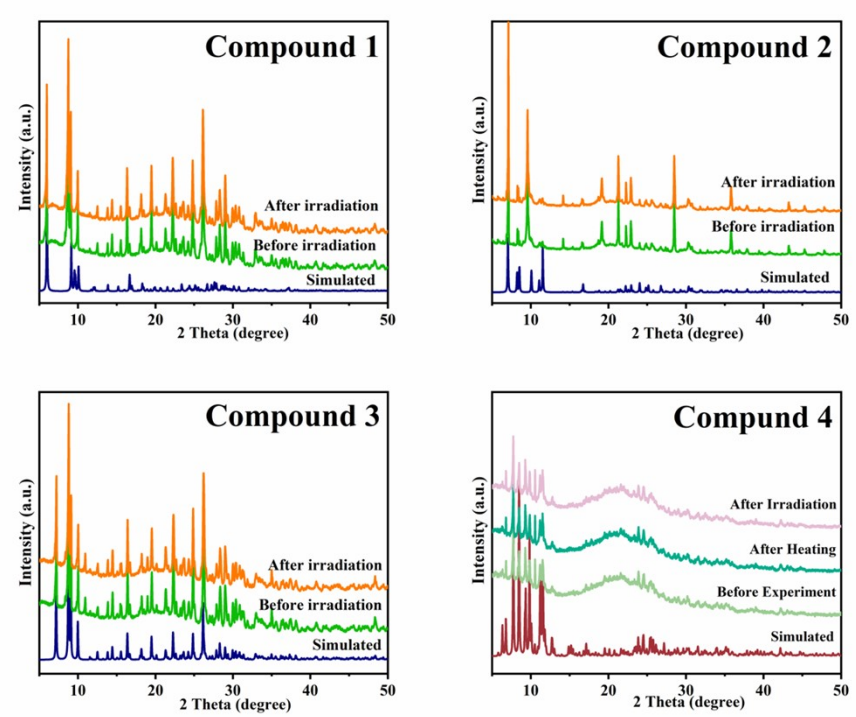

Fig. S13. The PXRD of compounds **1**–**4** before and after color change.

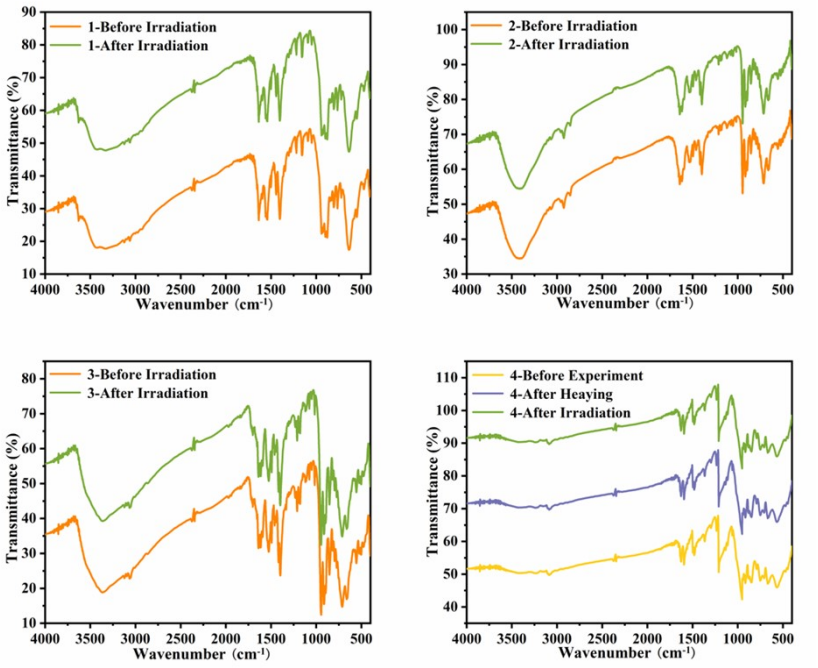

Fig. S14. The FT–IR spectra of compounds **1**–**4** before and after color change.

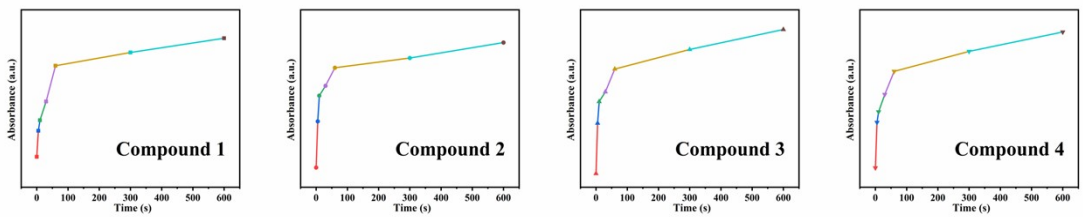

Fig. S15. Line chart of UV peak intensity along with irradiation time of compounds **1**–**4** (**1**-610 nm, **2**–625 nm, **3**–628 nm and **4**–614 nm).

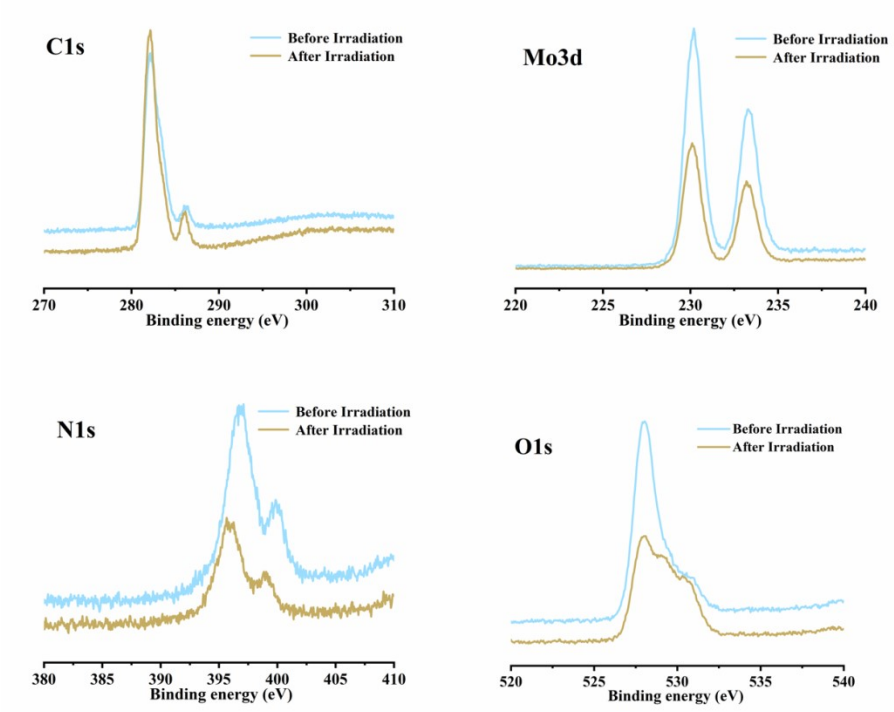

Fig. S16. XPS energy spectrum before irradiation (blue line) and after irradiation (yellow line) of compound **1**.

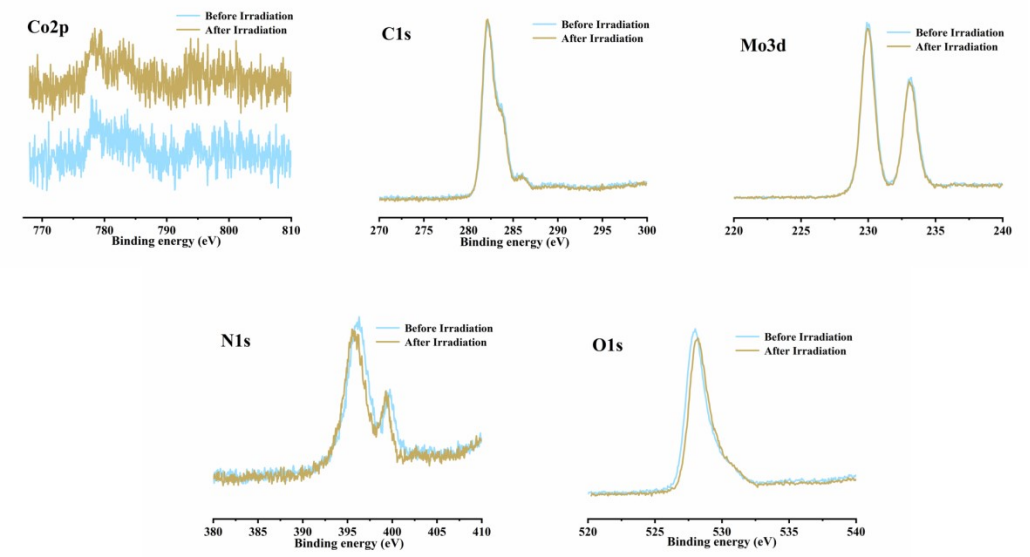

Fig. S17. XPS energy spectrum before irradiation (blue line) and after irradiation (yellow line) of compound **2**.

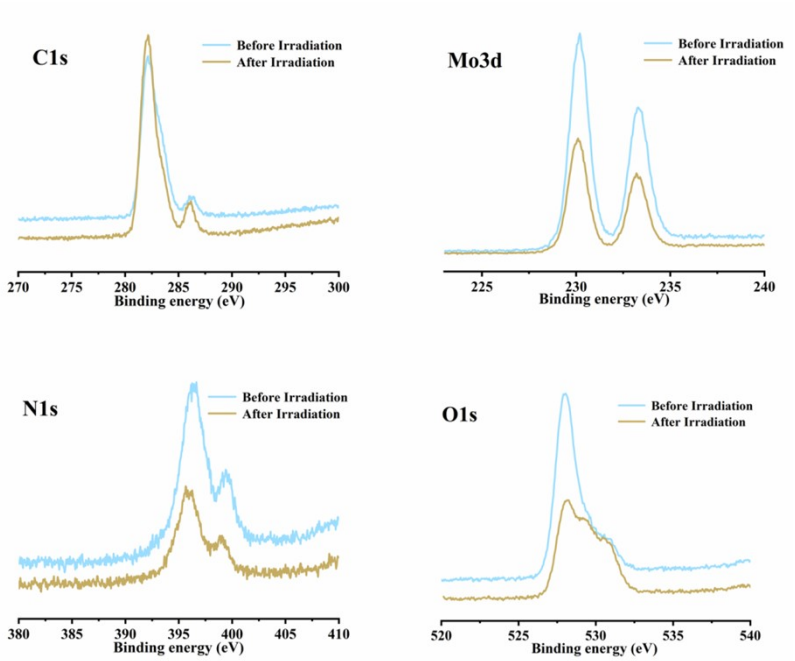

Fig. S18. XPS energy spectrum before irradiation (blue line) and after irradiation (yellow line) of compound **3**.

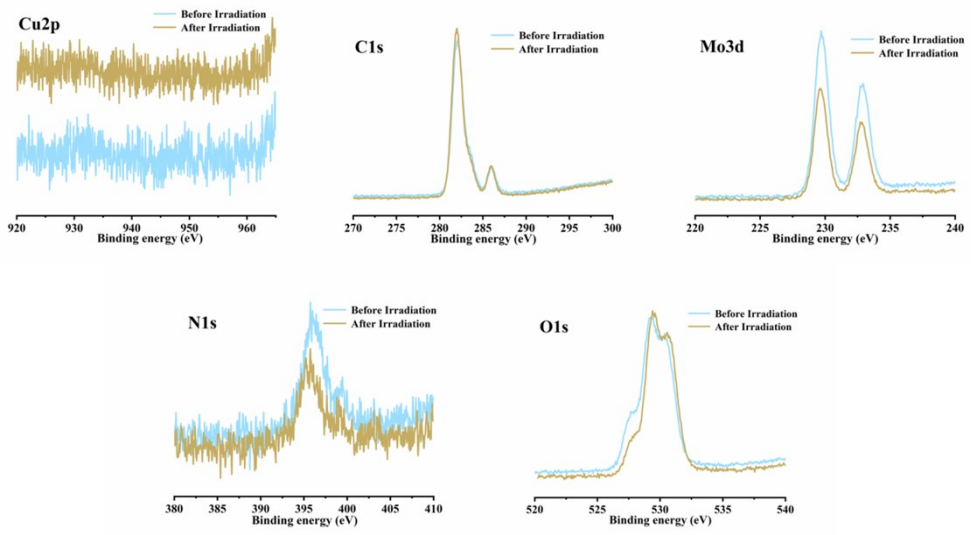

Fig. S19. XPS energy spectrum before irradiation (blue line) and after irradiation (yellow line) of compound **4**.

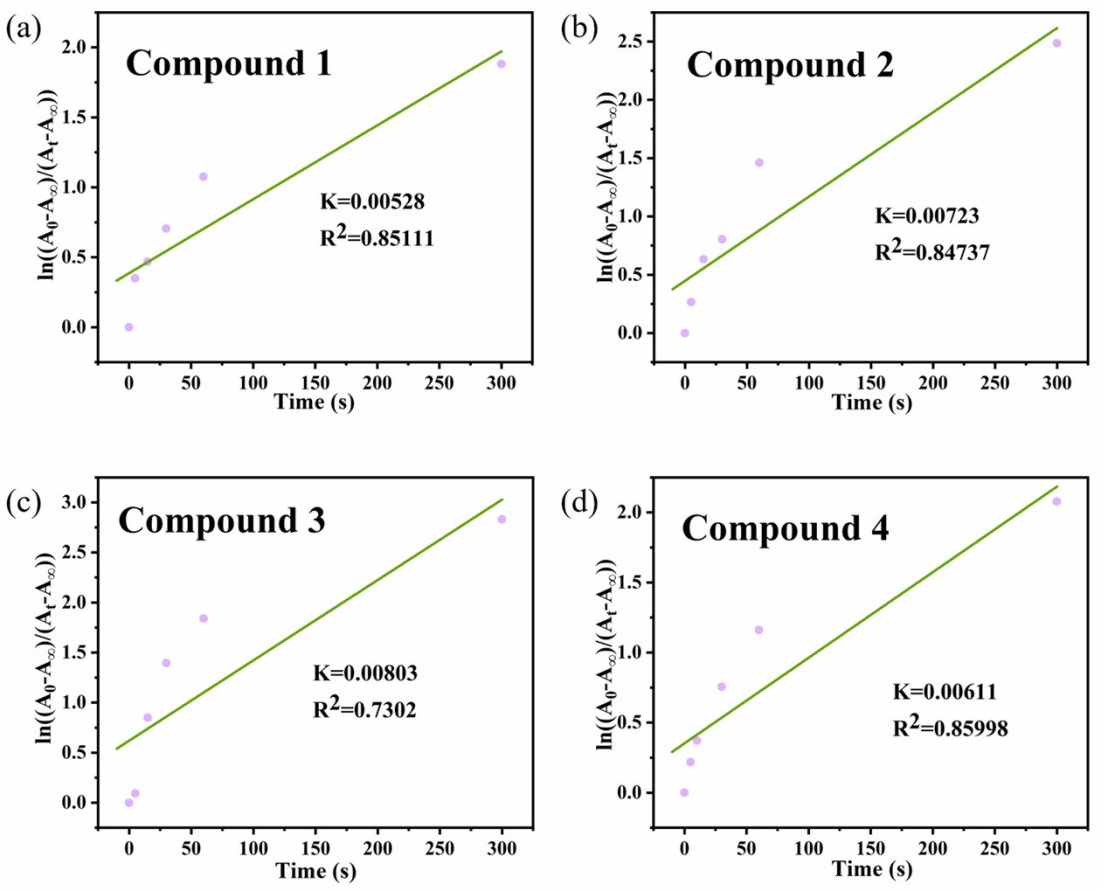

Fig. S20. Photochemical reaction kinetic plots of compound **1** (a), **2** (b), **3** (c) and **4** (d) monitored at 510, at 525, at 528 and at 514 nm, respectively.

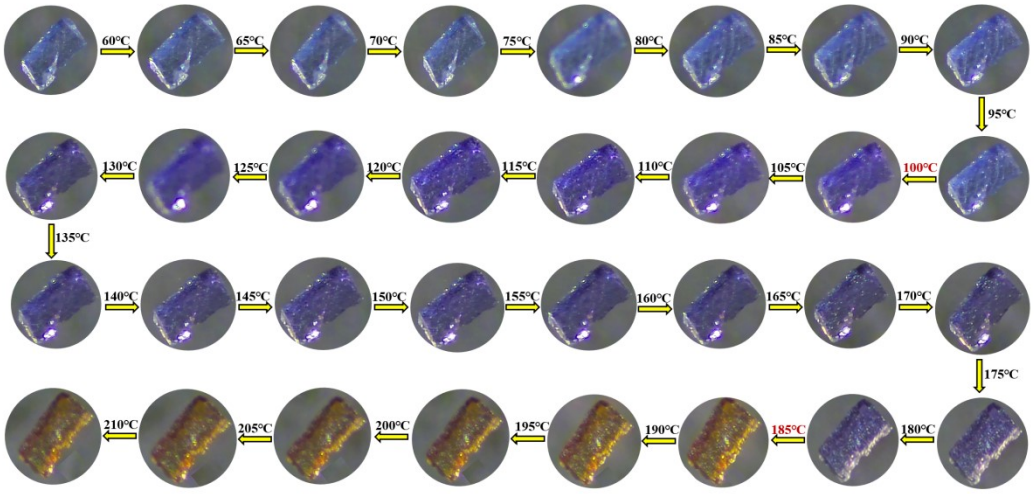

Fig. S21. Color change of compound **4** before and after heating.

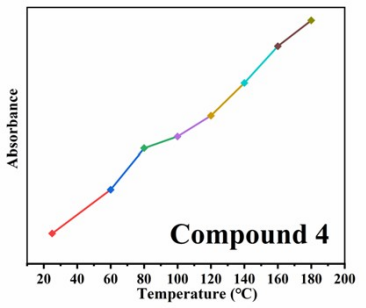

Figure S22. Line chart of UV peak intensity along with changing temperature of compound **4** (**4**–614 nm).

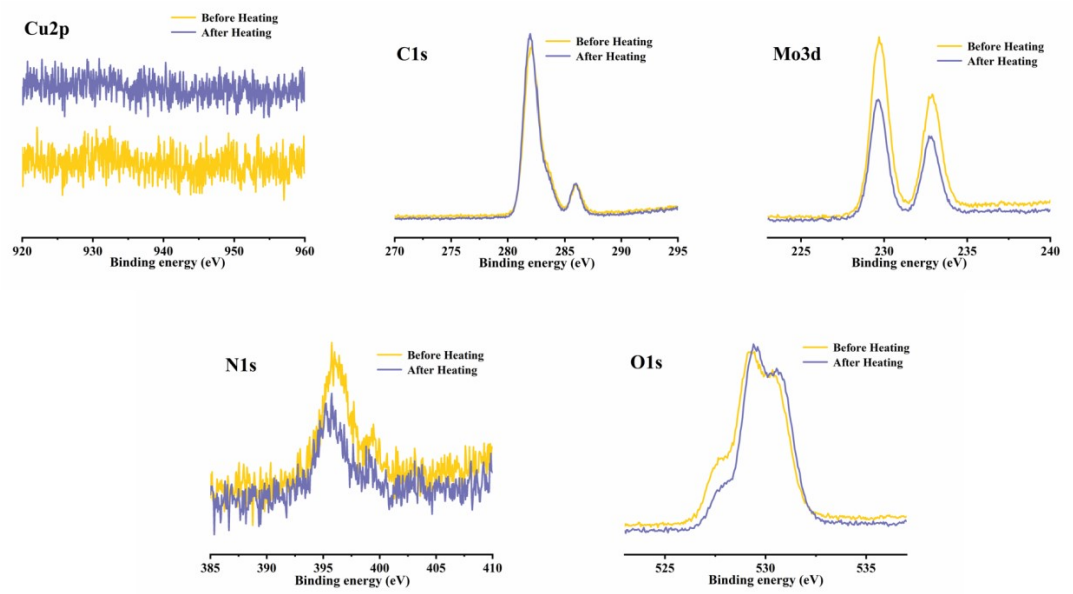

Fig. S23. XPS energy spectrum before heating (yellow line) and after irradiation (purple line) of compound **4**.

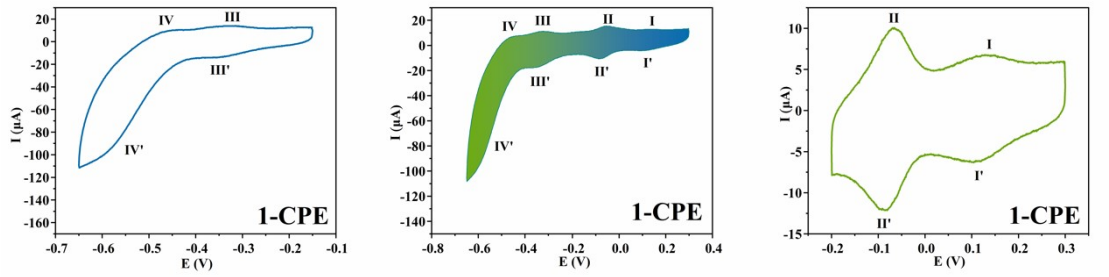

Fig. S24. Cyclic voltammograms of **1**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at 20 $mV \cdot s^{-1}$ scan rates.

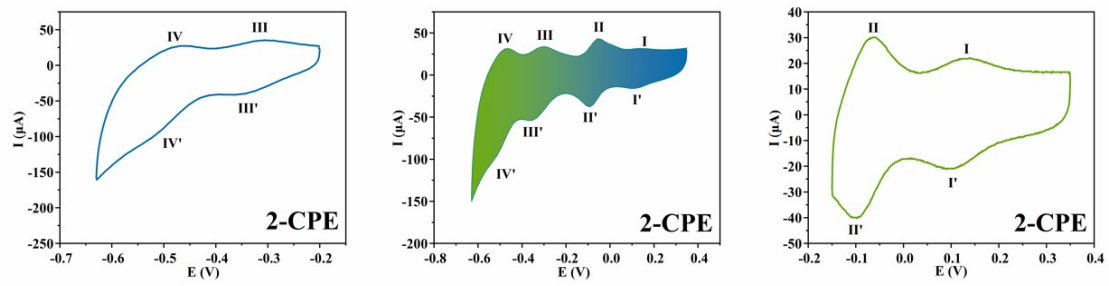

Fig. S25. Cyclic voltammograms of **2**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at 20 mV·s^{-1} scan rates.

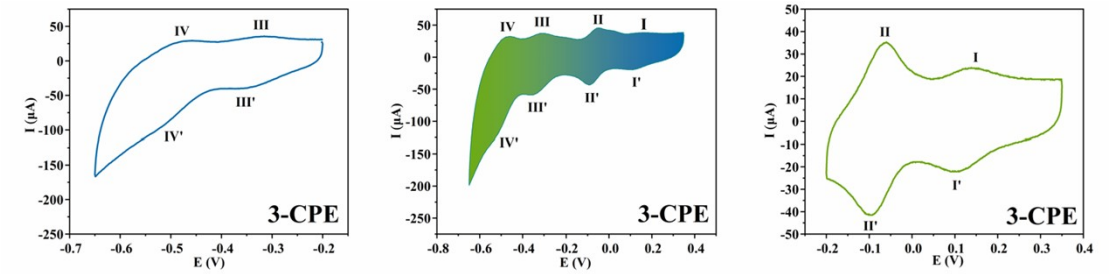

Fig. S26. Cyclic voltammograms of **3**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at 20 mV·s^{-1} scan rates.

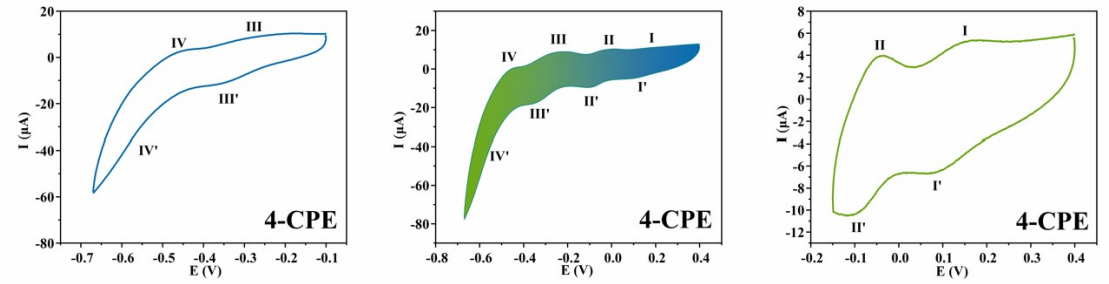

Fig. S27. Cyclic voltammograms of **4**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at 20 mV·s^{-1} scan rates.

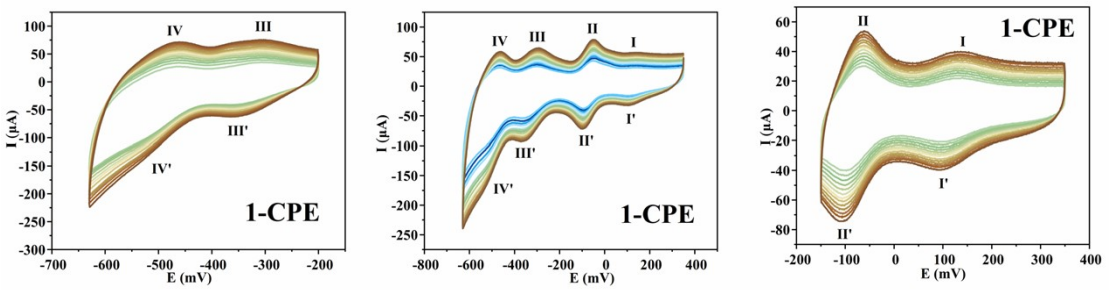

Fig. S28. Cyclic voltammograms of **1**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous

solution at different scan rates (20-500 mV·s^{-1}).

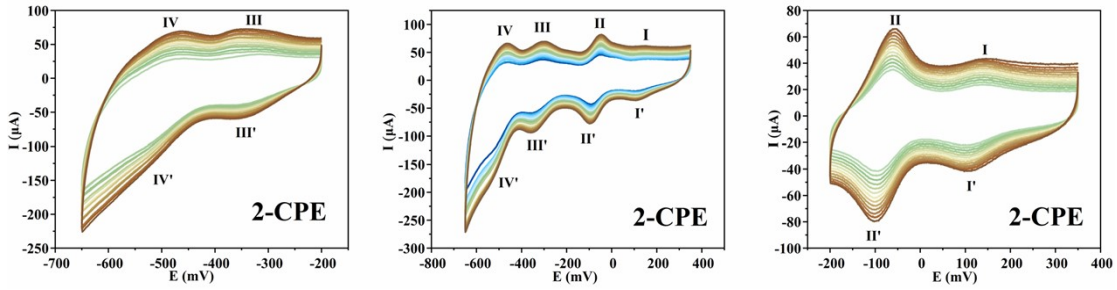

Fig. S29. Cyclic voltammograms of **2**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at different scan rates (20-500 mV·s^{-1}).

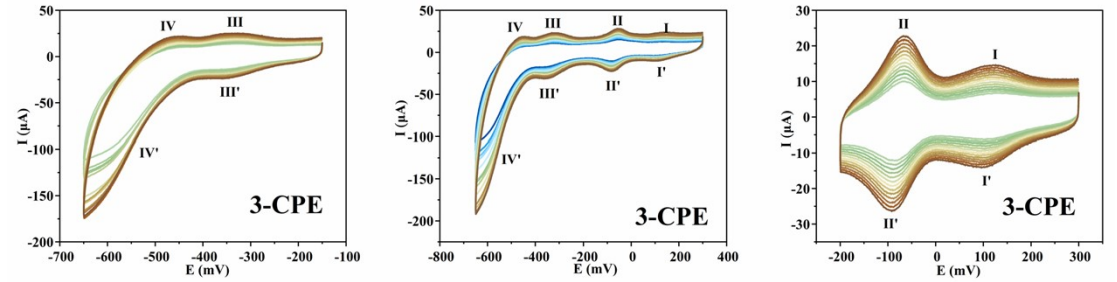

Fig. S30. Cyclic voltammograms of **3**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at different scan rates (20-500 mV·s^{-1}).

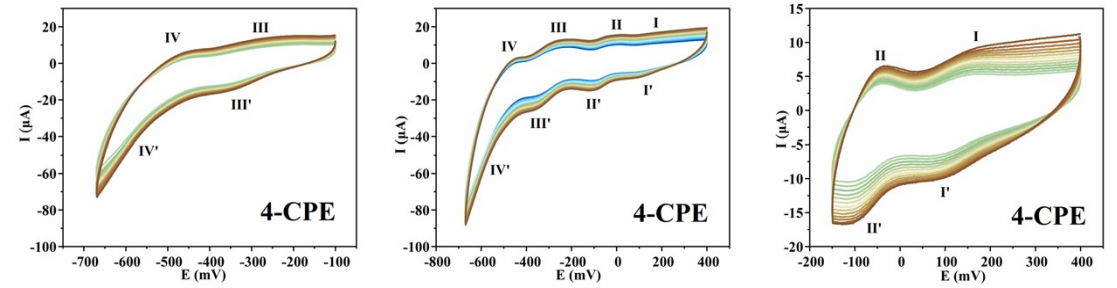

Fig. S31. Cyclic voltammograms of **4**–CPE in 0.1 M H_2SO_4 +0.5 M Na_2SO_4 aqueous solution at different scan rates (20-500 mV·s^{-1}).

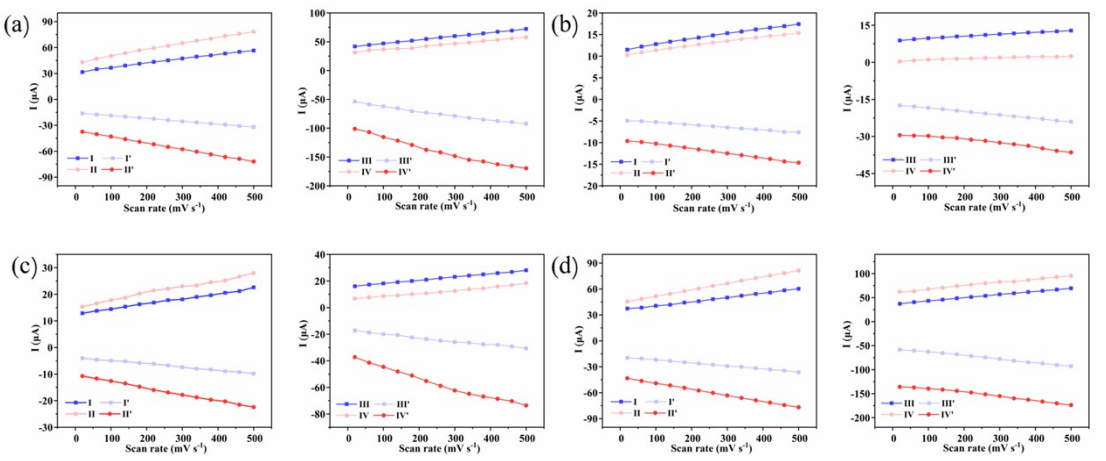

Fig. S32. (a-d) The plots of the anodic and cathodic peak currents *vs* scan rates of compounds **1**–**4**.

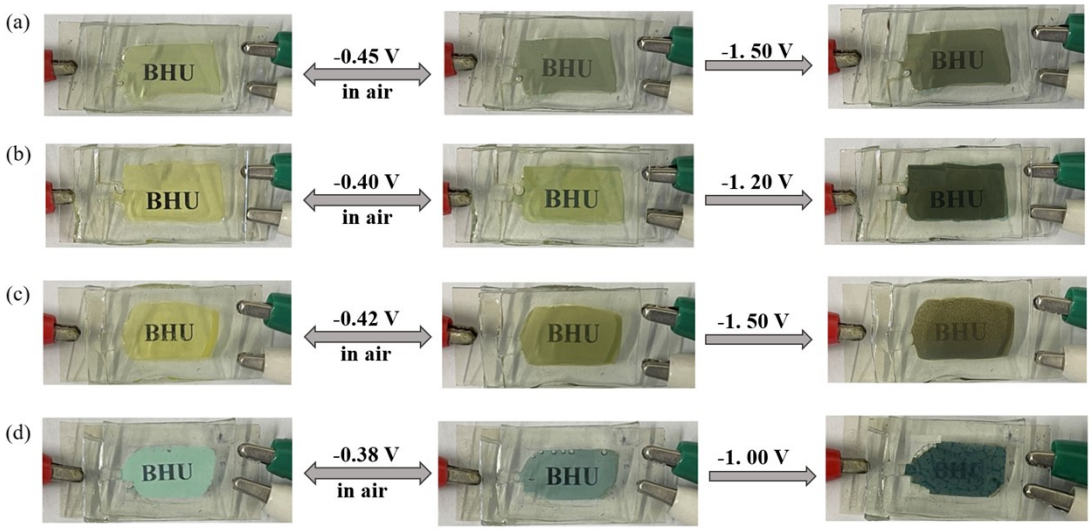

Fig. S33. (a-d) Color change of **1**/**2**/**3**/**4**–ECD under voltage application.

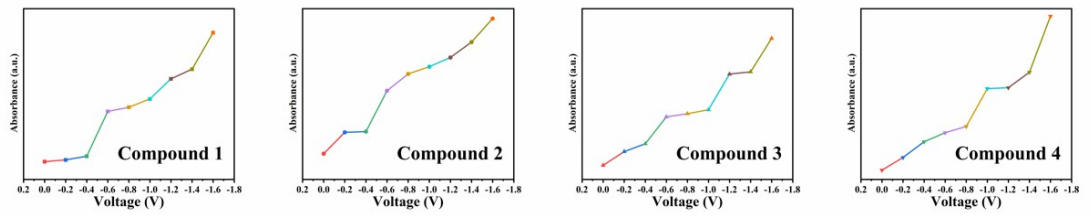

Fig. S34. Line chart of UV peak intensity along with applied voltage of compounds **1**–**4** (**1**-610 nm, **2**–625 nm, **3**–628 nm and **4**–614 nm).

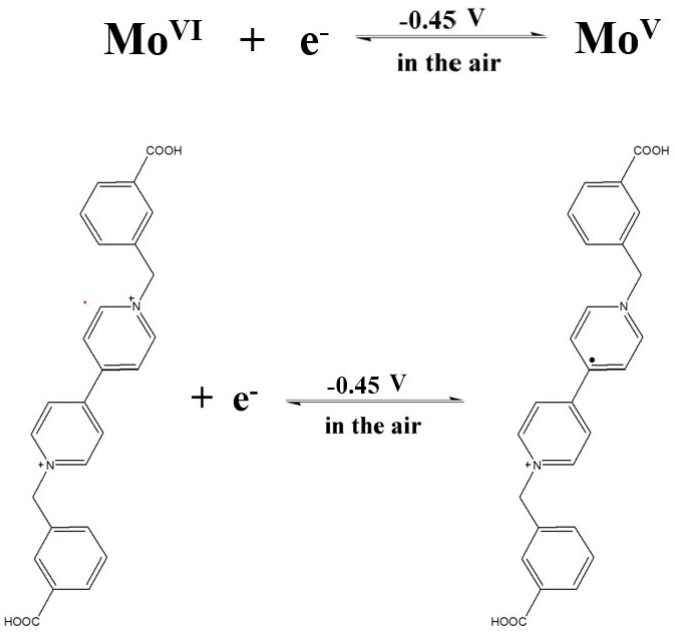

Fig. S35. The electron transfer reactions of compound **1** in redox process.

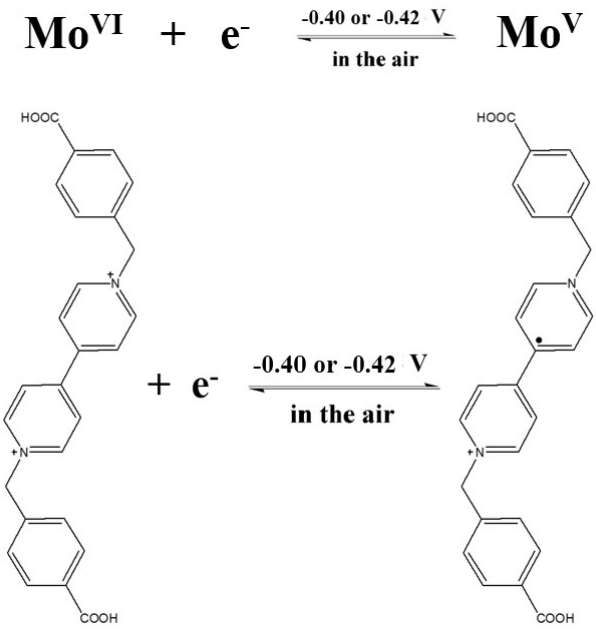

Fig. S36. The electron transfer reactions of compounds **2** and **3** in redox process.

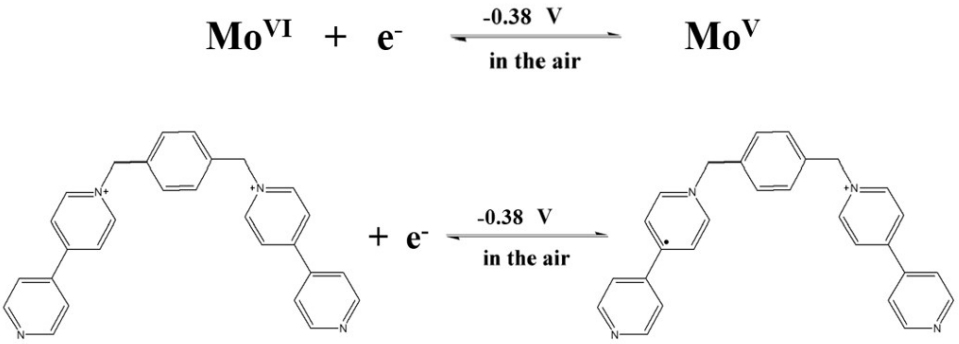

Fig. S37. The electron transfer reactions of compound **4** in redox process.

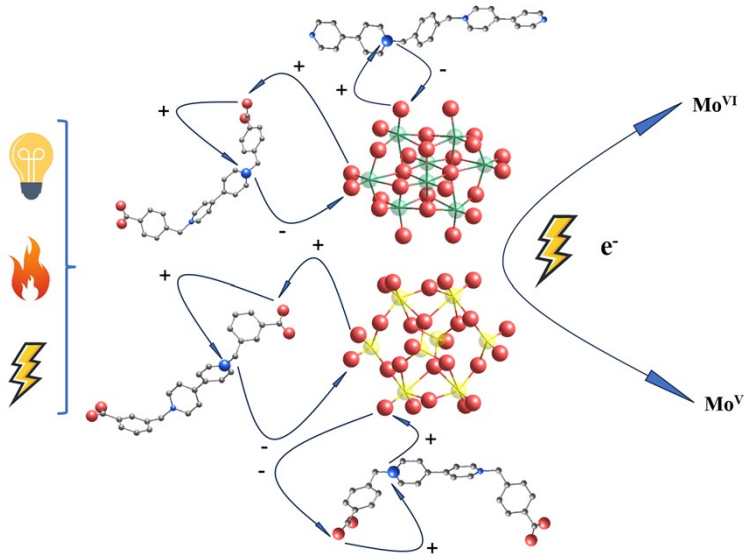

Fig. S38. The ET process of compounds **1**–**4**.

Table. S2. Selected bond lengths (Å) for compounds **1**–**4**.

Compound **1**					
Mo3	O14	1.795(2)	C15	C11	1.485(5)
Mo3	O12	1.776(2)	C15	C14	1.384(5)
Mo3	O7	1.770(2)	C10	C11	1.387(5)
Mo3	O13	1.700(2)	C10	C9	1.370(5)
Mo1	O16[1]	1.932(2)	C16	C17	1.370(5)
Mo1	O14[1]	2.352(2)	C11	C12	1.385(5)
Mo1	O8	1.923(2)	C14	C18	1.363(5)
Mo1	O6	1.695(2)	O2	C1	1.197(5)
Mo1	O5	1.698(2)	C7	C6	1.383(5)
Mo1	O7	2.333(2)	C7	C8	1.504(5)
Mo4	O16	1.891(2)	C7	C4	1.373(5)
Mo4	O14	2.352(2)	C2	C4	1.388(5)
Mo4	O11	1.910(2)	C2	C3	1.382(5)

Mo4	O12[1]	2.422(2)	C2	C1	1.481(5)
Mo4	O17	1.699(3)	C6	C5	1.389(5)
Mo4	O15	1.702(3)	C12	C13	1.357(6)
O8	Mo2	1.876(2)	C19	C20	1.512(6)
O11	Mo2	1.886(3)	C20	C21	1.366(6)
O10	Mo2	1.697(3)	C20	C25	1.388(6)
N2	C17	1.338(5)	C5	C3	1.377(5)
N2	C18	1.337(5)	O4	C26	1.323(7)
N2	C19	1.480(5)	O3	C26	1.169(7)
N1	C9	1.339(4)	C21	C22	1.374(7)
N1	C8	1.504(5)	C25	C24	1.375(7)
N1	C13	1.341(5)	C26	C22	1.526(7)
O9	Mo2	1.684(3)	C23	C22	1.367(7)
O1	C1	1.334(5)	C23	C24	1.397(7)
C15	C16	1.383(5)			

Symmetry codes for **1**: [1]-X,2-Y,1-Z.

Compound **2**

Mo(2)	Mo(1)	3.2098(4)	Co(1)	O(2)	2.119(3)
Mo(2)	Mo(1)[1]	3.2097(4)	Co(1)	O(2)[5]	2.119(3)
Mo(2)	O(5)[1]	1.943(3)	Co(1)	O(2)[4]	2.119(3)
Mo(2)	O(5)	1.943(3)	Co(1)	O(2)[1]	2.119(3)
Mo(2)	O(10)	2.125(3)	O(2)	C(1)	1.250(5)
Mo(2)	O(10)[2]	2.374(3)	N(1)	C(9)	1.347(6)
Mo(2)	O(12)	1.754(4)	N(1)	C(13)	1.333(6)
Mo(2)	O(11)	1.683(4)	N(1)	C(8)	1.483(5)
Mo(1)	O(5)	1.999(3)	O(1)	C(1)	1.243(5)
Mo(1)	O(5)[3]	2.362(3)	C(11)	C(11)[3]	1.477(8)
Mo(1)	O(10)	2.3198(6)	C(11)	C(10)	1.386(6)
Mo(1)	O(6)	1.886(3)	C(11)	C(12)	1.382(6)
Mo(1)	O(7)	1.690(3)	C(9)	C(10)	1.373(6)
Mo(1)	O(4)	1.698(3)	C(1)	C(2)	1.496(6)
Mo(3)	O(10)	2.487(3)	C(7)	C(2)	1.386(6)
Mo(3)	O(12)[2]	2.290(4)	C(7)	C(6)	1.389(6)
Mo(3)	O(6)[1]	1.915(3)	C(4)	C(5)	1.375(6)
Mo(3)	O(6)	1.915(3)	C(4)	C(3)	1.378(6)
Mo(3)	O(9)	1.686(5)	C(2)	C(3)	1.381(6)
Mo(3)	O(8)	1.701(5)	C(6)	C(5)	1.383(6)
Co(1)	O(3)[4]	2.085(4)	C(5)	C(8)	1.506(6)
Co(1)	O(3)	2.085(4)	C(13)	C(12)	1.376(7)

Symmetry codes for **2**: [1]+X,1-Y,+Z; [2]1-X,1-Y,-Z; [3]1-X,+Y,-Z; [4]-X,1-Y,1-Z; [5]-X,+Y,1-Z.

Compound **3**

Mo4	O8	1.758(4)	N1	C13	1.345(9)
Mo4	O10	1.679(5)	C11	C12	1.411(9)
Mo4	O9	1.773(5)	C11	C10	1.368(8)

Mo4	O13	1.790(4)	C11	C14	1.475(8)
Mo1	O14	1.945(4)	C12	C13	1.369(10)
Mo1	O16	1.921(4)	C5	C6	1.388(9)
Mo1	O17	1.693(4)	C5	C4	1.391(9)
Mo1	O15	1.684(4)	C5	C8	1.503(9)
Mo1	O9[1]	2.303(4)	C20	C21	1.403(9)
Mo1	O13	2.335(4)	C20	C19	1.516(9)
Mo3	O16[1]	1.905(4)	C20	C25	1.363(8)
Mo3	O7	1.936(4)	C10	C9	1.366(9)
Mo3	O8	2.381(4)	C14	C15	1.391(8)
Mo3	O5	1.693(5)	C14	C18	1.375(9)
Mo3	O6	1.680(4)	O3	C26	1.308(9)
Mo3	O13[1]	2.380(4)	C15	C16	1.370(9)
Mo2	O14	1.852(4)	C21	C22	1.384(10)
Mo2	O7	1.853(4)	C6	C7	1.345(10)
Mo2	O11	1.691(5)	C4	C3	1.409(9)
Mo2	O12	1.693(5)	C1	C2	1.523(10)
N2	C16	1.343(8)	C25	C24	1.372(9)
N2	C19	1.501(8)	C23	C24	1.384(9)
N2	C17	1.331(8)	C23	C26	1.504(10)
O2	C1	1.304(10)	C23	C22	1.384(9)
O1	C1	1.194(9)	C17	C18	1.353(9)
O4	C26	1.193(9)	C3	C2	1.378(10)
N1	C9	1.315(8)	C2	C7	1.361(10)
N1	C8	1.514(8)			

Symmetry codes for **3**: [1]2-X,2-Y,1-Z.

Compound **4**

Mo6	Mo5	3.2187(6)	Mo16	O13	1.692(5)
Mo6	Mo7	3.2179(6)	Mo2	O46	2.359(4)
Mo6	O36	1.948(3)	Mo2	O40[2]	2.369(5)
Mo6	O33	2.147(3)	Mo2	O47	1.828(5)
Mo6	O33[1]	2.380(4)	Mo2	O51	1.982(5)
Mo6	O32	1.952(3)	Mo2	O49	1.624(6)
Mo6	O38	1.746(3)	Mo2	O52	1.773(6)
Mo6	O35	1.685(4)	Cu1	N5	2.027(4)
Mo5	O36[1]	2.342(4)	Cu1	N1[3]	2.036(4)
Mo5	O33	2.319(3)	Cu1	O53	2.389(4)
Mo5	O32	1.989(3)	Cu1	N4	2.010(4)
Mo5	O28	1.899(3)	Cu1	N7	2.039(4)
Mo5	O27	1.707(4)	O46	Mo1A	2.235(12)
Mo5	O30	1.704(4)	O45	Mo1A[2]	2.307(8)
Mo13	Mo11	3.2005(7)	O40	Mo2A[2]	2.162(7)
Mo13	O14	2.382(4)	O41	Mo1A	2.169(17)
Mo13	O23	1.966(4)	N5	C43	1.346(6)

Mo13	O10	1.949(4)	N5	C44	1.324(7)
Mo13	O19	2.130(4)	N1	C5	1.334(7)
Mo13	O22	1.677(4)	N1	C1	1.323(7)
Mo13	O17	1.749(4)	N4	C28	1.343(6)
Mo7	O36	1.990(3)	N4	C24	1.330(6)
Mo7	O33	2.335(3)	O47	Mo1A	1.66(2)
Mo7	O32[1]	2.355(4)	O47	Mo2A	2.150(11)
Mo7	O34	1.902(3)	N7	C30	1.341(6)
Mo7	O39	1.706(4)	N7	C29	1.338(6)
Mo7	O37	1.685(4)	N2	C10	1.312(7)
Mo4	Mo1	3.213(4)	N2	C11	1.495(6)
Mo4	O46[2]	2.340(4)	N2	C6	1.339(7)
Mo4	O46	2.147(4)	N8	C37	1.341(6)
Mo4	O45	1.948(4)	N8	C38	1.337(6)
Mo4	O40	1.741(4)	N8	C39	1.499(6)
Mo4	O43	1.704(4)	O51	Mo2A	1.767(7)
Mo4	O41	1.942(4)	O42	Mo1A	1.824(14)
Mo8	O33	2.445(3)	C2	C3	1.372(7)
Mo8	O38[1]	2.275(4)	C2	C1	1.391(7)
Mo8	O28	1.924(4)	O44	Mo1A	1.743(10)
Mo8	O34	1.910(4)	C49	C51	1.353(7)
Mo8	O29	1.705(3)	C49	C48	1.390(7)
Mo8	O31	1.705(4)	N6	C51	1.327(7)
Mo12	Mo15	3.2047(7)	N6	C53	1.501(7)
Mo12	O14	2.126(4)	N6	C52	1.338(7)
Mo12	O18	1.953(4)	O49	Mo2A	1.980(12)
Mo12	O19	2.370(4)	C43	C46	1.367(7)
Mo12	O4	1.938(4)	C26	C21	1.486(7)
Mo12	O9	1.754(4)	C26	C25	1.356(7)
Mo12	O11	1.693(4)	C26	C27	1.381(8)
Mo1	Mo2	3.216(7)	C3	C8	1.479(6)
Mo1	O46	2.405(6)	C3	C4	1.367(7)
Mo1	O45[2]	2.337(5)	C46	C47	1.373(7)
Mo1	O41	1.943(6)	C5	C4	1.379(6)
Mo1	O47	1.979(7)	C44	C45	1.381(7)
Mo1	O42	1.641(7)	C30	C32	1.378(7)
Mo1	O44	1.690(5)	C47	C45	1.383(6)
Mo10	O23	1.984(4)	C47	C48	1.494(7)
Mo10	O18	2.318(4)	C33	C34	1.483(7)
Mo10	O19	2.351(3)	C33	C32	1.368(7)
Mo10	O21	1.885(4)	C33	C31	1.388(7)
Mo10	O26	1.702(4)	C35	C37	1.355(7)
Mo10	O25	1.700(4)	C35	C34	1.400(7)
Mo11	O10	1.980(4)	C38	C36	1.358(7)

Mo11	O19	2.357(3)	C10	C9	1.364(7)
Mo11	O4	2.387(4)	C34	C36	1.387(7)
Mo11	O5	1.911(4)	C8	C7	1.382(7)
Mo11	O6	1.686(4)	C8	C9	1.379(7)
Mo11	O1	1.703(4)	C7	C6	1.369(7)
Mo15	O14	2.325(4)	C48	C50	1.375(8)
Mo15	O10	2.374(4)	C31	C29	1.379(7)
Mo15	O4	1.980(4)	C15	C16	1.381(9)
Mo15	O8	1.897(5)	C15	C14	1.376(9)
Mo15	O2	1.696(4)	C15	C18	1.503(9)
Mo15	O3	1.699(4)	C28	C27	1.396(7)
Mo3	O46	2.323(3)	C11	C12	1.495(8)
Mo3	O45	2.002(4)	C12	C13	1.377(8)
Mo3	O41[2]	2.332(4)	C12	C17	1.380(8)
Mo3	O51	1.888(4)	N3	C19	1.323(8)
Mo3	O48	1.696(5)	N3	C18	1.494(7)
Mo3	O50	1.702(5)	N3	C23	1.299(9)
Mo14	O14	2.363(4)	C21	C20	1.372(9)
Mo14	O23	2.331(4)	C21	C22	1.361(9)
Mo14	O18	1.995(4)	C40	C42	1.389(8)
Mo14	O16	1.897(4)	C40	C39	1.494(7)
Mo14	O15	1.691(4)	C40	C41	1.389(8)
Mo14	O24	1.695(4)	C24	C25	1.376(7)
Mo9	O19	2.392(4)	C55	C54	1.375(8)
Mo9	O9	2.272(4)	C55	C56	1.390(8)
Mo9	O21	1.944(4)	C16	C17	1.375(9)
Mo9	O5	1.912(4)	O52	Mo2A	1.435(10)
Mo9	O20	1.697(4)	C42	C41[4]	1.371(8)
Mo9	O7	1.697(5)	C53	C54	1.501(8)
Mo16	O14	2.457(4)	C54	C56[5]	1.378(8)
Mo16	O17	2.280(4)	C50	C52	1.367(8)
Mo16	O16	1.920(4)	C19	C20	1.377(8)
Mo16	O8	1.917(4)	C13	C14	1.359(9)
Mo16	O12	1.689(5)	C22	C23	1.401(10)

Symmetry codes for **4**: [1]2-X,-Y,2-Z; [2]-1-X,-Y,1-Z; [3]-1+X,+Y,-1+Z; [4]-1-X,1-Y,1-Z; [5]1-X,-Y,-Z.

Table. S3. Selected bond angles (°) for compounds **1**–**4**.

Compound **1**							
O12	Mo3	O14	110.12(11)	C13	N1	C8	119.1(3)
O7	Mo3	O14	109.36(12)	C16	C15	C11	120.7(3)
O7	Mo3	O12	109.40(11)	C16	C15	C14	118.4(3)
O13	Mo3	O14	108.97(12)	C14	C15	C11	120.8(3)
O13	Mo3	O12	109.98(12)	C9	C10	C11	119.6(3)

O13	Mo3	O7	109.00(12)	C17	C16	C15	119.6(3)
O16[1]	Mo1	O14[1]	72.22(8)	C10	C11	C15	119.3(3)
O16[1]	Mo1	O7	81.34(9)	C12	C11	C15	122.3(3)
O8	Mo1	O16[1]	147.34(10)	C12	C11	C10	118.3(3)
O8	Mo1	O14[1]	80.15(9)	N1	C9	C10	120.5(3)
O8	Mo1	O7	75.36(10)	C18	C14	C15	119.6(3)
O6	Mo1	O16[1]	98.77(11)	N2	C17	C16	120.6(3)
O6	Mo1	O14[1]	163.20(11)	C6	C7	C8	119.7(4)
O6	Mo1	O8	103.14(12)	C4	C7	C6	119.4(4)
O6	Mo1	O5	105.23(12)	C4	C7	C8	120.9(3)
O6	Mo1	O7	88.54(11)	N2	C18	C14	121.0(3)
O5	Mo1	O16[1]	99.36(11)	C4	C2	C1	118.0(3)
O5	Mo1	O14[1]	90.44(10)	C3	C2	C4	119.8(3)
O5	Mo1	O8	97.91(12)	C3	C2	C1	122.3(4)
O5	Mo1	O7	165.85(10)	C7	C6	C5	120.1(4)
O7	Mo1	O14[1]	76.25(9)	C7	C8	N1	110.7(3)
O16	Mo4	O14	72.89(9)	C13	C12	C11	120.0(4)
O16	Mo4	O11	144.71(10)	N2	C19	C20	110.7(3)
O16	Mo4	O12[1]	78.19(9)	C21	C20	C19	120.1(4)
O14	Mo4	O12[1]	75.87(8)	C21	C20	C25	119.4(4)
O11	Mo4	O14	80.58(9)	C25	C20	C19	120.5(4)
O11	Mo4	O12[1]	73.00(9)	C3	C5	C6	120.2(4)
O17	Mo4	O16	99.48(11)	C7	C4	C2	120.8(3)
O17	Mo4	O14	165.37(11)	N1	C13	C12	120.7(4)
O17	Mo4	O11	100.69(12)	C5	C3	C2	119.7(4)
O17	Mo4	O12[1]	90.47(11)	O1	C1	C2	114.3(4)
O17	Mo4	O15	104.82(14)	O2	C1	O1	122.3(4)
O15	Mo4	O16	102.58(12)	O2	C1	C2	123.4(4)
O15	Mo4	O14	89.21(12)	C20	C21	C22	121.3(5)
O15	Mo4	O11	99.85(12)	C24	C25	C20	120.2(4)
O15	Mo4	O12[1]	164.23(11)	O4	C26	C22	109.7(6)
Mo4	O16	Mo1[1]	120.73(11)	O3	C26	O4	125.9(6)
Mo3	O14	Mo1[1]	133.13(12)	O3	C26	C22	124.4(6)
Mo3	O14	Mo4	132.95(12)	C22	C23	C24	120.6(5)
Mo4	O14	Mo1[1]	89.86(7)	C21	C22	C26	115.9(5)
Mo2	O8	Mo1	126.56(13)	C23	C22	C21	119.3(4)
Mo2	O11	Mo4	126.62(13)	C23	C22	C26	124.7(5)
Mo3	O12	Mo4[1]	129.72(12)	C25	C24	C23	119.1(5)
Mo3	O7	Mo1	130.72(12)	O8	Mo2	O11	135.06(10)
C17	N2	C19	120.3(3)	O10	Mo2	O8	102.26(12)
C18	N2	C17	120.5(3)	O10	Mo2	O11	105.77(12)
C18	N2	C19	119.2(3)	O9	Mo2	O8	103.38(13)
C9	N1	C8	120.0(3)	O9	Mo2	O11	101.76(13)
C9	N1	C13	120.9(3)	O9	Mo2	O10	106.00(15)

Symmetry codes for **1**: [1]-X,2-Y,1-Z.

Compound **2**

Mo(1)[1]	Mo(2)	Mo(1)	91.153(16)	O(8)	Mo(3)	O(10)	158.9(2)
O(5)[1]	Mo(2)	Mo(1)	124.93(8)	O(8)	Mo(3)	O(12)[2]	90.2(2)
O(5)	Mo(2)	Mo(1)	36.07(7)	O(8)	Mo(3)	O(6)	103.04(9)
O(5)[1]	Mo(2)	Mo(1)[1]	36.07(7)	O(8)	Mo(3)	O(6)[1]	103.04(9)
O(5)	Mo(2)	Mo(1)[1]	124.93(8)	O(3)[4]	Co(1)	O(3)	180.0
O(5)[1]	Mo(2)	O(5)	150.36(15)	O(3)[4]	Co(1)	O(2)[4]	92.43(12)
O(5)	Mo(2)	O(10)	78.71(8)	O(3)[4]	Co(1)	O(2)	87.57(12)
O(5)[1]	Mo(2)	O(10)	78.71(8)	O(3)[4]	Co(1)	O(2)[1]	87.57(11)
O(5)[1]	Mo(2)	O(10)[2]	78.00(8)	O(3)	Co(1)	O(2)[4]	87.57(12)
O(5)	Mo(2)	O(10)[2]	78.00(8)	O(3)	Co(1)	O(2)[5]	87.57(12)
O(10)	Mo(2)	Mo(1)	46.230(16)	O(3)[4]	Co(1)	O(2)[5]	92.43(12)
O(10)[2]	Mo(2)	Mo(1)[1]	86.12(6)	O(3)	Co(1)	O(2)	92.43(12)
O(10)[2]	Mo(2)	Mo(1)	86.12(6)	O(3)	Co(1)	O(2)[1]	92.43(12)
O(10)	Mo(2)	Mo(1)[1]	46.229(16)	O(2)[4]	Co(1)	O(2)[1]	83.78(19)
O(10)	Mo(2)	O(10)[2]	75.69(14)	O(2)	Co(1)	O(2)[4]	180.00(14)
O(12)	Mo(2)	Mo(1)[1]	132.45(3)	O(2)	Co(1)	O(2)[1]	96.22(19)
O(12)	Mo(2)	Mo(1)	132.44(3)	O(2)[4]	Co(1)	O(2)[5]	96.22(19)
O(12)	Mo(2)	O(5)[1]	96.39(8)	O(2)[1]	Co(1)	O(2)[5]	180.00(15)
O(12)	Mo(2)	O(5)	96.39(8)	O(2)	Co(1)	O(2)[5]	83.78(19)
O(12)	Mo(2)	O(10)	155.85(16)	Mo(2)	O(5)	Mo(1)	109.02(12)
O(12)	Mo(2)	O(10)[2]	80.16(15)	Mo(2)	O(5)	Mo(1)[3]	109.91(11)
O(11)	Mo(2)	Mo(1)	90.76(10)	Mo(1)	O(5)	Mo(1)[3]	104.25(11)
O(11)	Mo(2)	Mo(1)[1]	90.76(10)	Mo(2)	O(10)	Mo(2)[2]	104.31(14)
O(11)	Mo(2)	O(5)	101.29(8)	Mo(2)	O(10)	Mo(1)	92.35(9)
O(11)	Mo(2)	O(5)[1]	101.29(8)	Mo(2)	O(10)	Mo(1)[1]	92.35(9)
O(11)	Mo(2)	O(10)[2]	175.54(17)	Mo(2)[2]	O(10)	Mo(3)	91.99(12)
O(11)	Mo(2)	O(10)	99.85(17)	Mo(2)	O(10)	Mo(3)	163.70(17)
O(11)	Mo(2)	O(12)	104.3(2)	Mo(1)	O(10)	Mo(2)[2]	97.64(8)
O(5)	Mo(1)	Mo(2)	34.91(7)	Mo(1)[1]	O(10)	Mo(2)[2]	97.64(8)
O(5)[3]	Mo(1)	Mo(2)	78.61(6)	Mo(1)[1]	O(10)	Mo(1)	162.37(17)
O(5)	Mo(1)	O(5)[3]	71.41(11)	Mo(1)[1]	O(10)	Mo(3)	85.36(9)
O(5)	Mo(1)	O(10)	73.06(11)	Mo(1)	O(10)	Mo(3)	85.36(9)
O(10)	Mo(1)	Mo(2)	41.42(9)	Mo(2)	O(12)	Mo(3)[2]	119.14(19)
O(10)	Mo(1)	O(5)[3]	71.55(10)	Mo(1)	O(6)	Mo(3)	118.11(14)
O(6)	Mo(1)	Mo(2)	119.28(8)	C(1)	O(2)	Co(1)	130.5(3)
O(6)	Mo(1)	O(5)[3]	84.18(11)	C(9)	N(1)	C(8)	119.1(4)
O(6)	Mo(1)	O(5)	146.62(11)	C(13)	N(1)	C(9)	120.7(4)
O(6)	Mo(1)	O(10)	77.88(12)	C(13)	N(1)	C(8)	120.2(4)
O(7)	Mo(1)	Mo(2)	85.79(10)	C(10)	C(11)	C(11)[3]	120.9(5)
O(7)	Mo(1)	O(5)	96.87(13)	C(12)	C(11)	C(11)[3]	121.1(5)
O(7)	Mo(1)	O(5)[3]	164.26(12)	C(12)	C(11)	C(10)	118.0(4)
O(7)	Mo(1)	O(10)	95.31(13)	N(1)	C(9)	C(10)	120.4(4)

O(7)	Mo(1)	O(6)	101.88(13)	O(2)	C(1)	C(2)	117.9(4)
O(7)	Mo(1)	O(4)	105.15(16)	O(1)	C(1)	O(2)	124.6(4)
O(4)	Mo(1)	Mo(2)	135.78(11)	O(1)	C(1)	C(2)	117.2(4)
O(4)	Mo(1)	O(5)	100.87(13)	C(2)	C(7)	C(6)	119.9(4)
O(4)	Mo(1)	O(5)[3]	87.75(13)	C(5)	C(4)	C(3)	120.9(4)
O(4)	Mo(1)	O(10)	159.30(15)	C(7)	C(2)	C(1)	120.2(4)
O(4)	Mo(1)	O(6)	100.54(15)	C(3)	C(2)	C(1)	120.9(4)
O(12)[2]	Mo(3)	O(10)	68.71(12)	C(3)	C(2)	C(7)	118.9(4)
O(6)[1]	Mo(3)	O(10)	73.22(8)	C(5)	C(6)	C(7)	120.9(4)
O(6)	Mo(3)	O(10)	73.22(8)	C(9)	C(10)	C(11)	120.1(4)
O(6)[1]	Mo(3)	O(12)[2]	77.42(9)	C(4)	C(5)	C(6)	118.6(4)
O(6)	Mo(3)	O(12)[2]	77.42(9)	C(4)	C(5)	C(8)	118.2(4)
O(6)[1]	Mo(3)	O(6)	143.51(16)	C(6)	C(5)	C(8)	123.1(4)
O(9)	Mo(3)	O(10)	94.62(19)	C(4)	C(3)	C(2)	120.8(4)
O(9)	Mo(3)	O(12)[2]	163.3(2)	N(1)	C(13)	C(12)	120.8(4)
O(9)	Mo(3)	O(6)	98.29(10)	C(13)	C(12)	C(11)	120.0(4)
O(9)	Mo(3)	O(6)[1]	98.28(10)	N(1)	C(8)	C(5)	112.6(3)
O(9)	Mo(3)	O(8)	106.5(3)				

Symmetry codes for **2**: [1]+X,1-Y,+Z; [2]1-X,1-Y,-Z; [3]1-X,+Y,-Z; [4]-X,1-Y,1-Z; [5]-X,+Y,1-Z.

Compound **3**

O8	Mo4	O9	112.7(2)	Mo4	O9	Mo1[1]	127.5(2)
O8	Mo4	O13	108.7(2)	C9	N1	C8	119.5(5)
O10	Mo4	O8	107.5(2)	C9	N1	C13	120.7(6)
O10	Mo4	O9	107.5(3)	C13	N1	C8	119.6(6)
O10	Mo4	O13	108.7(3)	C12	C11	C14	120.7(5)
O9	Mo4	O13	111.6(2)	C10	C11	C12	116.5(6)
O14	Mo1	O9[1]	75.09(17)	C10	C11	C14	122.8(5)
O14	Mo1	O13	82.62(17)	C13	C12	C11	119.6(6)
O16	Mo1	O14	149.90(18)	C6	C5	C4	119.9(6)
O16	Mo1	O9[1]	81.66(17)	C6	C5	C8	119.9(6)
O16	Mo1	O13	72.55(16)	C4	C5	C8	120.2(6)
O17	Mo1	O14	96.7(2)	C21	C20	C19	121.5(6)
O17	Mo1	O16	100.4(2)	C25	C20	C21	118.5(6)
O17	Mo1	O9[1]	163.2(2)	C25	C20	C19	120.0(6)
O17	Mo1	O13	91.0(2)	C9	C10	C11	121.6(6)
O15	Mo1	O14	101.6(2)	C15	C14	C11	122.1(5)
O15	Mo1	O16	97.3(2)	C18	C14	C11	122.0(5)
O15	Mo1	O17	105.8(2)	C18	C14	C15	115.9(6)
O15	Mo1	O9[1]	90.3(2)	Mo4	O13	Mo1	137.8(2)
O15	Mo1	O13	161.9(2)	Mo4	O13	Mo3[1]	132.3(2)
O9[1]	Mo1	O13	73.6(2)	Mo1	O13	Mo3[1]	89.75(15)
O16[1]	Mo3	O7	146.36(17)	C16	C15	C14	120.8(6)
O16[1]	Mo3	O8	79.84(17)	C22	C21	C20	120.2(6)
O16[1]	Mo3	O13[1]	71.73(16)	C7	C6	C5	120.3(7)

O7	Mo3	O8	76.42(17)	N1	C9	C10	120.6(6)
O7	Mo3	O13[1]	78.93(16)	N2	C16	C15	120.8(5)
O5	Mo3	O16[1]	101.0(2)	N2	C19	C20	111.9(5)
O5	Mo3	O7	96.7(2)	C5	C4	C3	118.0(6)
O5	Mo3	O8	166.3(2)	O2	C1	C2	111.0(7)
O5	Mo3	O13[1]	93.3(2)	O1	C1	O2	125.5(8)
O6	Mo3	O16[1]	102.3(2)	O1	C1	C2	123.5(7)
O6	Mo3	O7	100.6(2)	C20	C25	C24	121.9(6)
O6	Mo3	O8	88.7(2)	C24	C23	C26	117.8(6)
O6	Mo3	O5	104.4(3)	C22	C23	C24	119.7(6)
O6	Mo3	O13[1]	162.2(2)	C22	C23	C26	122.5(6)
O13[1]	Mo3	O8	73.80(19)	C25	C24	C23	119.8(6)
O14	Mo2	O7	130.95(18)	O4	C26	O3	124.7(7)
O11	Mo2	O14	108.1(2)	O4	C26	C23	123.9(6)
O11	Mo2	O7	103.4(2)	O3	C26	C23	111.4(7)
O11	Mo2	O12	106.7(3)	N2	C17	C18	121.5(6)
O12	Mo2	O14	102.3(2)	C23	C22	C21	119.9(6)
O12	Mo2	O7	103.5(2)	C17	C18	C14	121.7(6)
Mo2	O14	Mo1	126.0(2)	C5	C8	N1	111.6(5)
Mo3[1]	O16	Mo1	120.9(2)	C2	C3	C4	120.7(6)
Mo2	O7	Mo3	131.9(2)	N1	C13	C12	120.7(6)
Mo4	O8	Mo3	126.0(2)	C3	C2	C1	122.7(6)
C16	N2	C19	120.2(5)	C7	C2	C1	118.1(7)
C17	N2	C16	119.3(5)	C7	C2	C3	119.2(6)
C17	N2	C19	120.4(5)	C6	C7	C2	121.9(7)

Symmetry codes for **3**: [1]2-X,2-Y,1-Z.

Compound **4**

Mo7	Mo6	Mo5	91.393(14)	O20	Mo9	O19	92.05(18)
O36	Mo6	Mo5	124.56(9)	O20	Mo9	O9	162.23(19)
O36	Mo6	Mo7	35.62(9)	O20	Mo9	O21	97.5(2)
O36	Mo6	O33[1]	77.59(13)	O20	Mo9	O5	99.5(2)
O36	Mo6	O33	78.54(13)	O20	Mo9	O7	104.6(2)
O36	Mo6	O32	149.66(14)	O7	Mo9	O19	163.3(2)
O33[1]	Mo6	Mo5	86.18(8)	O7	Mo9	O9	93.1(2)
O33	Mo6	Mo5	46.05(9)	O7	Mo9	O21	101.0(2)
O33[1]	Mo6	Mo7	86.10(7)	O7	Mo9	O5	102.1(2)
O33	Mo6	Mo7	46.50(9)	O17	Mo16	O14	69.93(13)
O33	Mo6	O33[1]	76.19(14)	O16	Mo16	O14	74.27(16)
O32	Mo6	Mo5	35.63(9)	O16	Mo16	O17	77.52(17)
O32	Mo6	Mo7	124.74(9)	O8	Mo16	O14	73.45(16)
O32	Mo6	O33[1]	78.10(13)	O8	Mo16	O17	78.18(17)
O32	Mo6	O33	78.25(12)	O8	Mo16	O16	144.63(19)
O38	Mo6	Mo5	132.33(11)	O12	Mo16	O14	94.2(2)
O38	Mo6	Mo7	132.45(11)	O12	Mo16	O17	164.1(2)

O38	Mo6	O36	96.84(15)	O12	Mo16	O16	97.5(2)
O38	Mo6	O33[1]	80.39(14)	O12	Mo16	O8	98.9(2)
O38	Mo6	O33	156.58(15)	O12	Mo16	O13	106.0(3)
O38	Mo6	O32	96.72(15)	O13	Mo16	O14	159.8(2)
O35	Mo6	Mo5	90.24(13)	O13	Mo16	O17	89.9(2)
O35	Mo6	Mo7	90.01(13)	O13	Mo16	O16	102.9(2)
O35	Mo6	O36	101.30(17)	O13	Mo16	O8	102.3(2)
O35	Mo6	O33[1]	174.65(14)	O46	Mo2	Mo1	48.17(13)
O35	Mo6	O33	98.46(16)	O46	Mo2	O40[2]	69.67(14)
O35	Mo6	O32	101.21(17)	O40[2]	Mo2	Mo1	83.31(14)
O35	Mo6	O38	104.96(17)	O47	Mo2	Mo1	33.82(16)
O36[1]	Mo5	Mo6	78.54(8)	O47	Mo2	O46	77.96(17)
O33	Mo5	Mo6	41.80(7)	O47	Mo2	O40[2]	77.67(17)
O33	Mo5	O36[1]	71.77(12)	O47	Mo2	O51	145.80(19)
O32	Mo5	Mo6	34.86(9)	O51	Mo2	Mo1	122.45(17)
O32	Mo5	O36[1]	71.44(13)	O51	Mo2	O46	74.31(16)
O32	Mo5	O33	73.49(12)	O51	Mo2	O40[2]	74.22(19)
O28	Mo5	Mo6	119.49(11)	O49	Mo2	Mo1	90.9(3)
O28	Mo5	O36[1]	83.57(14)	O49	Mo2	O46	97.5(2)
O28	Mo5	O33	77.70(13)	O49	Mo2	O40[2]	166.6(2)
O28	Mo5	O32	146.44(15)	O49	Mo2	O47	104.0(3)
O27	Mo5	Mo6	135.06(13)	O49	Mo2	O51	99.1(2)
O27	Mo5	O36[1]	87.90(17)	O49	Mo2	O52	103.3(3)
O27	Mo5	O33	159.68(18)	O52	Mo2	Mo1	136.0(2)
O27	Mo5	O32	100.20(16)	O52	Mo2	O46	158.4(3)
O27	Mo5	O28	100.90(16)	O52	Mo2	O40[2]	89.2(2)
O30	Mo5	Mo6	87.03(14)	O52	Mo2	O47	102.2(2)
O30	Mo5	O36[1]	165.28(16)	O52	Mo2	O51	96.5(3)
O30	Mo5	O33	95.53(17)	N5	Cu1	N1[3]	87.38(16)
O30	Mo5	O32	98.24(16)	N5	Cu1	O53	91.52(16)
O30	Mo5	O28	101.33(17)	N5	Cu1	N7	176.81(18)
O30	Mo5	O27	104.6(2)	N1[3]	Cu1	O53	91.48(16)
O14	Mo13	Mo11	86.32(9)	N1[3]	Cu1	N7	90.50(16)
O23	Mo13	Mo11	125.70(11)	N4	Cu1	N5	90.72(15)
O23	Mo13	O14	77.93(14)	N4	Cu1	N1[3]	178.09(16)
O23	Mo13	O19	78.28(15)	N4	Cu1	O53	88.78(17)
O10	Mo13	Mo11	35.77(12)	N4	Cu1	N7	91.39(16)
O10	Mo13	O14	77.65(14)	N7	Cu1	O53	90.92(17)
O10	Mo13	O23	150.21(15)	Mo6	O36	Mo5[1]	110.39(15)
O10	Mo13	O19	79.32(15)	Mo6	O36	Mo7	109.61(16)
O19	Mo13	Mo11	47.43(9)	Mo7	O36	Mo5[1]	104.39(14)
O19	Mo13	O14	75.56(14)	Mo6	O33	Mo6[1]	103.81(13)
O22	Mo13	Mo11	90.15(15)	Mo6	O33	Mo5	92.16(11)
O22	Mo13	O14	174.15(18)	Mo6	O33	Mo7	91.67(12)

O22	Mo13	O23	100.48(18)	Mo6	O33	Mo8	164.59(17)
O22	Mo13	O10	102.08(18)	Mo6[1]	O33	Mo8	91.60(10)
O22	Mo13	O19	98.62(18)	Mo5	O33	Mo6[1]	97.38(12)
O22	Mo13	O17	105.1(2)	Mo5	O33	Mo7	163.55(17)
O17	Mo13	Mo11	131.76(13)	Mo5	O33	Mo8	86.07(11)
O17	Mo13	O14	80.74(16)	Mo7	O33	Mo6[1]	97.22(13)
O17	Mo13	O23	96.66(18)	Mo7	O33	Mo8	85.99(10)
O17	Mo13	O10	95.99(17)	Mo6	O32	Mo5	109.51(15)
O17	Mo13	O19	156.30(17)	Mo6	O32	Mo7[1]	110.11(15)
O36	Mo7	Mo6	34.77(10)	Mo5	O32	Mo7[1]	103.94(13)
O36	Mo7	O33	73.30(12)	Mo6	O38	Mo8[1]	118.15(16)
O36	Mo7	O32[1]	71.15(13)	Mo4	O46	Mo4[2]	104.37(13)
O33	Mo7	Mo6	41.82(7)	Mo4[2]	O46	Mo1	97.62(15)
O33	Mo7	O32[1]	71.77(12)	Mo4	O46	Mo1	89.59(18)
O32[1]	Mo7	Mo6	78.58(7)	Mo4	O46	Mo3	92.33(12)
O34	Mo7	Mo6	118.84(11)	Mo4[2]	O46	Mo2	94.89(16)
O34	Mo7	O36	145.79(15)	Mo4	O46	Mo2	160.52(19)
O34	Mo7	O33	77.02(13)	Mo4	O46	Mo1A	96.8(5)
O34	Mo7	O32[1]	83.76(14)	Mo3	O46	Mo4[2]	97.69(13)
O39	Mo7	Mo6	135.76(13)	Mo3	O46	Mo1	163.59(18)
O39	Mo7	O36	101.01(17)	Mo3	O46	Mo2	87.92(14)
O39	Mo7	O33	159.84(18)	Mo2	O46	Mo1	84.90(18)
O39	Mo7	O32[1]	88.07(18)	Mo1A	O46	Mo3	160.5(3)
O39	Mo7	O34	101.00(17)	Mo4	O45	Mo1[2]	112.6(2)
O37	Mo7	Mo6	85.38(14)	Mo4	O45	Mo3	109.51(15)
O37	Mo7	O36	96.99(17)	Mo4	O45	Mo1A[2]	106.6(4)
O37	Mo7	O33	94.50(18)	Mo3	O45	Mo1[2]	101.5(2)
O37	Mo7	O32[1]	163.75(16)	Mo3	O45	Mo1A[2]	109.4(5)
O37	Mo7	O34	101.97(19)	Mo5	O28	Mo8	116.61(17)
O37	Mo7	O39	105.5(2)	Mo7	O34	Mo8	117.63(17)
O46	Mo4	Mo1	48.47(14)	Mo13	O14	Mo16	91.39(12)
O46[2]	Mo4	Mo1	86.18(11)	Mo12	O14	Mo13	104.16(16)
O46	Mo4	O46[2]	75.63(13)	Mo12	O14	Mo15	92.00(14)
O45	Mo4	Mo1	126.65(15)	Mo12	O14	Mo14	92.17(14)
O45	Mo4	O46	78.21(14)	Mo12	O14	Mo16	164.43(18)
O45	Mo4	O46[2]	77.95(13)	Mo15	O14	Mo13	98.23(13)
O40	Mo4	Mo1	130.59(17)	Mo15	O14	Mo14	163.15(19)
O40	Mo4	O46	157.07(17)	Mo15	O14	Mo16	86.17(13)
O40	Mo4	O46[2]	81.44(16)	Mo14	O14	Mo13	96.56(13)
O40	Mo4	O45	97.11(17)	Mo14	O14	Mo16	85.45(13)
O40	Mo4	O41	96.38(18)	Mo4	O40	Mo2[2]	113.9(2)
O43	Mo4	Mo1	89.59(15)	Mo4	O40	Mo2A[2]	123.7(4)
O43	Mo4	O46[2]	174.12(17)	Mo13	O23	Mo10	110.21(19)
O43	Mo4	O46	98.50(18)	Mo13	O23	Mo14	110.75(16)

O43	Mo4	O45	101.43(18)	Mo10	O23	Mo14	103.09(15)
O43	Mo4	O40	104.4(2)	Mo4	O41	Mo1	111.6(2)
O43	Mo4	O41	100.61(18)	Mo4	O41	Mo3[2]	110.11(16)
O41	Mo4	Mo1	34.21(15)	Mo4	O41	Mo1A	105.6(4)
O41	Mo4	O46	79.09(15)	Mo1	O41	Mo3[2]	103.5(2)
O41	Mo4	O46[2]	78.09(14)	C43	N5	Cu1	119.5(4)
O41	Mo4	O45	150.32(16)	C44	N5	Cu1	122.1(3)
O38[1]	Mo8	O33	69.86(11)	C44	N5	C43	118.0(4)
O28	Mo8	O33	74.12(12)	Mo13	O10	Mo11	109.09(18)
O28	Mo8	O38[1]	77.53(15)	Mo13	O10	Mo15	110.41(16)
O34	Mo8	O33	74.15(12)	Mo11	O10	Mo15	104.01(15)
O34	Mo8	O38[1]	77.80(15)	Mo12	O18	Mo10	111.18(17)
O34	Mo8	O28	144.90(15)	Mo12	O18	Mo14	110.16(19)
O29	Mo8	O33	161.61(17)	Mo14	O18	Mo10	103.19(15)
O29	Mo8	O38[1]	91.76(17)	Mo13	O19	Mo12	104.40(16)
O29	Mo8	O28	102.10(17)	Mo13	O19	Mo10	92.44(13)
O29	Mo8	O34	103.23(17)	Mo13	O19	Mo11	90.85(13)
O31	Mo8	O33	93.92(15)	Mo13	O19	Mo9	162.84(18)
O31	Mo8	O38[1]	163.68(15)	Mo12	O19	Mo9	92.74(12)
O31	Mo8	O28	96.71(19)	Mo10	O19	Mo12	96.74(13)
O31	Mo8	O34	100.1(2)	Mo10	O19	Mo11	163.70(18)
O31	Mo8	O29	104.4(2)	Mo10	O19	Mo9	86.15(12)
O14	Mo12	Mo15	46.48(9)	Mo11	O19	Mo12	97.89(13)
O14	Mo12	O19	75.88(14)	Mo11	O19	Mo9	86.02(12)
O18	Mo12	Mo15	125.30(12)	C5	N1	Cu1[4]	120.8(3)
O18	Mo12	O14	78.82(15)	C1	N1	Cu1[4]	120.5(3)
O18	Mo12	O19	77.65(14)	C1	N1	C5	118.7(4)
O19	Mo12	Mo15	86.72(9)	C28	N4	Cu1	122.9(3)
O4	Mo12	Mo15	35.55(13)	C24	N4	Cu1	119.9(3)
O4	Mo12	O14	78.32(15)	C24	N4	C28	116.8(4)
O4	Mo12	O18	150.14(15)	Mo2	O47	Mo1	115.2(3)
O4	Mo12	O19	78.35(14)	Mo1A	O47	Mo2A	120.6(5)
O9	Mo12	Mo15	132.35(13)	Mo12	O4	Mo11	110.63(17)
O9	Mo12	O14	155.64(16)	Mo12	O4	Mo15	109.77(19)
O9	Mo12	O18	96.13(18)	Mo15	O4	Mo11	103.57(15)
O9	Mo12	O19	79.76(16)	Mo12	O9	Mo9	117.22(18)
O9	Mo12	O4	96.81(18)	C30	N7	Cu1	120.8(3)
O11	Mo12	Mo15	90.83(15)	C29	N7	Cu1	121.5(3)
O11	Mo12	O14	100.00(19)	C29	N7	C30	117.8(4)
O11	Mo12	O18	101.12(18)	Mo10	O21	Mo9	115.58(19)
O11	Mo12	O19	175.84(18)	Mo13	O17	Mo16	117.93(19)
O11	Mo12	O4	101.54(18)	Mo11	O5	Mo9	115.9(2)
O11	Mo12	O9	104.4(2)	Mo14	O16	Mo16	118.0(2)
Mo4	Mo1	Mo2	87.39(14)	C10	N2	C11	119.9(5)

O46	Mo1	Mo4	41.94(11)	C10	N2	C6	119.4(4)
O46	Mo1	Mo2	46.94(14)	C6	N2	C11	120.6(5)
$O45^2$	Mo1	Mo4	78.39(14)	C37	N8	C39	116.8(4)
$O45^2$	Mo1	Mo2	85.76(19)	C38	N8	C37	120.1(4)
$O45^2$	Mo1	O46	69.81(18)	C38	N8	C39	123.1(4)
O41	Mo1	Mo4	34.19(14)	Mo3	O51	Mo2	114.2(2)
O41	Mo1	Mo2	119.8(2)	Mo2A	O51	Mo3	128.0(5)
O41	Mo1	O46	72.8(2)	Mo15	O8	Mo16	118.0(2)
O41	Mo1	$O45^2$	72.49(19)	C3	C2	C1	120.9(5)
O41	Mo1	O47	143.3(3)	C51	C49	C48	119.5(5)
O47	Mo1	Mo4	116.1(3)	C51	N6	C53	121.0(5)
O47	Mo1	Mo2	30.94(15)	C51	N6	C52	120.5(5)
O47	Mo1	O46	74.2(2)	C52	N6	C53	118.4(5)
O47	Mo1	$O45^2$	81.4(2)	N5	C43	C46	122.2(5)
O42	Mo1	Mo4	140.5(3)	C25	C26	C21	122.1(5)
O42	Mo1	Mo2	130.1(3)	C25	C26	C27	117.7(5)
O42	Mo1	O46	160.1(3)	C27	C26	C21	120.2(5)
O42	Mo1	$O45^2$	90.8(2)	C2	C3	C8	121.1(5)
O42	Mo1	O41	106.3(3)	C4	C3	C2	117.7(4)
O42	Mo1	O47	99.3(3)	C4	C3	C8	121.2(5)
O42	Mo1	O44	107.1(3)	C43	C46	C47	119.8(5)
O44	Mo1	Mo4	85.5(2)	N6	C51	C49	121.5(5)
O44	Mo1	Mo2	85.2(3)	N1	C5	C4	123.0(5)
O44	Mo1	O46	92.6(3)	N5	C44	C45	122.9(5)
O44	Mo1	$O45^2$	161.8(3)	N7	C30	C32	122.5(5)
O44	Mo1	O41	98.6(3)	C46	C47	C45	118.2(5)
O44	Mo1	O47	98.5(3)	C46	C47	C48	121.1(4)
O23	Mo10	O18	72.02(14)	C45	C47	C48	120.7(5)
O23	Mo10	O19	72.77(14)	C32	C33	C34	120.5(4)
O18	Mo10	O19	71.56(13)	C32	C33	C31	117.9(5)
O21	Mo10	O23	146.28(16)	C31	C33	C34	121.5(5)
O21	Mo10	O18	84.10(16)	C37	C35	C34	119.4(5)
O21	Mo10	O19	77.34(15)	C44	C45	C47	118.8(5)
O26	Mo10	O23	96.90(18)	N8	C37	C35	121.5(5)
O26	Mo10	O18	164.29(16)	N8	C38	C36	121.0(5)
O26	Mo10	O19	94.80(17)	N2	C10	C9	122.2(6)
O26	Mo10	O21	100.8(2)	C35	C34	C33	120.6(5)
O25	Mo10	O23	103.0(2)	C36	C34	C33	121.8(5)
O25	Mo10	O18	89.36(18)	C36	C34	C35	117.6(5)
O25	Mo10	O19	160.89(18)	C7	C8	C3	121.3(5)
O25	Mo10	O21	100.1(2)	C9	C8	C3	122.4(5)
O25	Mo10	O26	104.3(2)	C9	C8	C7	116.4(5)
O10	Mo11	Mo13	35.14(10)	C6	C7	C8	120.8(5)
O10	Mo11	O19	73.33(14)	C38	C36	C34	120.2(5)

O10	Mo11	O4	71.32(14)	C33	C32	C30	119.9(5)
O19	Mo11	Mo13	41.72(9)	N1	C1	C2	120.6(5)
O19	Mo11	O4	70.61(13)	C49	C48	C47	121.7(5)
O4	Mo11	Mo13	78.45(9)	C50	C48	C49	118.0(5)
O5	Mo11	Mo13	118.24(12)	C50	C48	C47	120.3(5)
O5	Mo11	O10	145.24(16)	C29	C31	C33	119.5(5)
O5	Mo11	O19	76.53(15)	C16	C15	C18	121.9(6)
O5	Mo11	O4	82.70(16)	C14	C15	C16	118.1(6)
O6	Mo11	Mo13	86.24(16)	C14	C15	C18	119.9(6)
O6	Mo11	O10	98.54(19)	N4	C28	C27	122.6(5)
O6	Mo11	O19	94.96(18)	N2	C11	C12	113.9(5)
O6	Mo11	O4	164.05(18)	C13	C12	C11	120.7(6)
O6	Mo11	O5	100.9(2)	C13	C12	C17	118.7(6)
O6	Mo11	O1	104.5(2)	C17	C12	C11	120.6(6)
O1	Mo11	Mo13	136.94(18)	C19	N3	C18	120.3(6)
O1	Mo11	O10	101.8(2)	C23	N3	C19	121.5(6)
O1	Mo11	O19	160.45(19)	C23	N3	C18	117.9(6)
O1	Mo11	O4	89.86(18)	C20	C21	C26	120.8(5)
O1	Mo11	O5	100.8(2)	C22	C21	C26	122.6(6)
O14	Mo15	Mo12	41.52(10)	C22	C21	C20	116.6(6)
O14	Mo15	O10	71.20(13)	C42	C40	C39	119.3(5)
O10	Mo15	Mo12	78.78(9)	C41	C40	C42	118.5(5)
O4	Mo15	Mo12	34.68(11)	C41	C40	C39	122.0(5)
O4	Mo15	O14	72.80(15)	N4	C24	C25	123.3(5)
O4	Mo15	O10	71.59(14)	N7	C29	C31	122.4(5)
O8	Mo15	Mo12	118.57(13)	C26	C25	C24	120.4(5)
O8	Mo15	O14	77.06(16)	C3	C4	C5	119.0(5)
O8	Mo15	O10	82.68(17)	C54	C55	C56	120.1(5)
O8	Mo15	O4	145.23(17)	C17	C16	C15	121.2(6)
O2	Mo15	Mo12	135.03(17)	C26	C27	C28	119.2(5)
O2	Mo15	O14	159.11(19)	C41^{5}	C42	C40	120.2(6)
O2	Mo15	O10	87.92(18)	N2	C6	C7	120.8(5)
O2	Mo15	O4	100.4(2)	N6	C53	C54	112.1(5)
O2	Mo15	O8	101.7(2)	C55	C54	C53	121.4(6)
O2	Mo15	O3	104.8(2)	C55	C54	C56^{6}	119.2(6)
O3	Mo15	Mo12	86.88(17)	C56^{6}	C54	C53	119.4(6)
O3	Mo15	O14	95.85(18)	C52	C50	C48	120.1(6)
O3	Mo15	O10	165.29(18)	C54^{6}	C56	C55	120.7(6)
O3	Mo15	O4	98.3(2)	C40	C39	N8	115.5(4)
O3	Mo15	O8	101.6(2)	C10	C9	C8	120.5(6)
O46	Mo3	O41^{2}	71.34(12)	N3	C19	C20	119.7(7)
O45	Mo3	O46	73.07(13)	C42^{5}	C41	C40	121.2(6)
O45	Mo3	O41^{2}	71.62(14)	C14	C13	C12	121.1(6)
O51	Mo3	O46	76.84(16)	C13	C14	C15	121.0(7)

O51	Mo3	O45	146.08(16)	N6	C52	C50	120.3(6)
O51	Mo3	O41[2]	84.28(17)	C21	C20	C19	121.3(6)
O48	Mo3	O46	95.5(2)	C16	C17	C12	119.9(6)
O48	Mo3	O45	95.8(2)	N3	C18	C15	111.0(5)
O48	Mo3	O41[2]	163.8(2)	C21	C22	C23	120.4(7)
O48	Mo3	O51	102.4(2)	N3	C23	C22	120.3(7)
O48	Mo3	O50	105.3(3)	O46	Mo1A	O45[2]	73.4(3)
O50	Mo3	O46	158.9(2)	O41	Mo1A	O46	72.6(3)
O50	Mo3	O45	101.07(19)	O41	Mo1A	O45[2]	69.4(3)
O50	Mo3	O41[2]	87.5(2)	O47	Mo1A	O46	85.0(8)
O50	Mo3	O51	101.4(2)	O47	Mo1A	O45[2]	89.3(6)
O23	Mo14	O14	71.80(13)	O47	Mo1A	O41	152.5(7)
O18	Mo14	O14	72.45(14)	O47	Mo1A	O42	105.0(6)
O18	Mo14	O23	71.53(14)	O47	Mo1A	O44	109.8(7)
O16	Mo14	O14	77.00(16)	O42	Mo1A	O46	158.3(6)
O16	Mo14	O23	83.76(17)	O42	Mo1A	O45[2]	87.3(4)
O16	Mo14	O18	145.32(16)	O42	Mo1A	O41	91.6(8)
O15	Mo14	O14	94.87(18)	O44	Mo1A	O46	97.2(4)
O15	Mo14	O23	163.85(19)	O44	Mo1A	O45[2]	158.1(9)
O15	Mo14	O18	96.1(2)	O44	Mo1A	O41	89.1(7)
O15	Mo14	O16	102.5(2)	O44	Mo1A	O42	97.3(8)
O15	Mo14	O24	104.3(2)	O47	Mo2A	O40[2]	76.4(2)
O24	Mo14	O14	160.41(19)	O51	Mo2A	O40[2]	83.9(3)
O24	Mo14	O23	88.62(18)	O51	Mo2A	O47	136.5(5)
O24	Mo14	O18	101.1(2)	O51	Mo2A	O49	94.4(4)
O24	Mo14	O16	102.2(2)	O49	Mo2A	O40[2]	146.5(6)
O9	Mo9	O19	70.27(14)	O49	Mo2A	O47	82.4(5)
O21	Mo9	O19	75.29(15)	O52	Mo2A	O40[2]	107.8(6)
O21	Mo9	O9	76.77(16)	O52	Mo2A	O47	101.0(4)
O5	Mo9	O19	75.62(15)	O52	Mo2A	O51	121.9(8)
O5	Mo9	O9	78.31(16)	O52	Mo2A	O49	101.4(4)
O5	Mo9	O21	146.63(18)				

Symmetry codes for **4**: [1]2-X,-Y,2-Z; [2]-1-X,-Y,1-Z; [3]-1+X,+Y,-1+Z; [4]1+X,+Y,1+Z; [5]-1-X,1-Y,1-Z; [6]1-X,-Y,-Z.

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