Supporting Information

Photocatalyst based on transition metal-Schiff base ligand and V-doped Kegging-type polyoxometalate for efficient and stable CO_2 reduction

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1. Experimental section

1.1 Synthesis

2.0 g of 2,6-Diacetylpyridine was dissolved in 140 mL alcohol solution, which was added 5.34 g of semicarbazide hydrochlorie and 3.93 g of CH_3COONa. The mixture was stirred while an appropriate amount of deionized water was added to dissolve the solid particles completely. The mixed solution was heated at 40 °C for 4 hours without cooling. White solid formed in the solution, which was then filtered and washed with a dilute solution of sodium hydroxide in ethanol (a few drops of 2 M sodium hydroxide solution were added to the ethanol). The resulting yellowish powder was dried.[1]

1.2 Materials and Physical Property Research

2, 6-diacetylpyridine disemicarbazone (DAPSC) was synthesized according to the known literature method. Chemicals, reagents, and analyses: All chemicals (in addition to DAPSC) were used as purchased without purification. The Bruker D8X diffractometer with monochromatized Cu-Kα (λ = 0.15406 Å) radiation (from 5° to 50°) can determine PXRD patterns. The Nicolet Impact 410 FTIR spectrometer can obtain IR spectra (4000-400 cm^{-1}). The Diamond thermogravimetric analyzer can confirm the Thermogravimetric (TG) measurements, with the temperature rising from 25 ℃ to 1000 ℃ in the N_2 atmosphere (heating rate=10 ℃ min^{-1}). The SHIMADZU UV-2600 spectrophotometer can get the UV-vis diffuse reflectance spectra, with a wavelength range from 200-800 nm. X-ray photoelectron spectroscopy was performed with Thermo Escalab 250 XI electron spectrometer.

1.3 X-ray crystallography

The crystal XRD data of compounds **1**, and **2** was collected at 296(3) K on Bruker Apex II CCD with Mo-Kα radiation (λ = 0.71073 Å). The SHELX software package was utilized to resolve and refine the structure of compounds through the direct method and full-matrix least-squares method on F^2 in the SHELX-2018/3 program package. In addition, the non-H atoms were refined by anisotropic thermal parameters. The detailed crystallographic data of two compounds are summarized in Table S1. Main bond lengths and bond angles of compounds **1**, and **2** were provided in Tables S2-S3.

1.4 Mott–Schottky plot measurements

All electrochemical measurements (Mott–Schottky plot, Photocurrent) were carried out via a conventional three-electrode system in a 0.2 M Na_2SO_4 aqueous solution (pH = 6.8). The conductive glass, carbon rod and saturated Ag/AgCl electrode were considered as the working electrode, counter electrode, and reference electrode, respectively. The preparation of the working electrode was given as follows: catalyst of 2 mg was ground to powder and then dispersed in anhydrous ethanol (990 μL) in the presence of 10 μL 5% Nafion solution by ultrasonication to form a homogeneous ink. Subsequently, 200 μL of the ink was deposited onto the carbon cloth (S = 1 cm × 2 cm), and dried at room temperature for Mott–Schottky spots measurements. The Mott–Schottky plots were measured over an alternating current (AC) frequency of 1500 Hz, 2000 Hz and 2500 Hz, and three electrodes were immersed in the 0.2

M Na_2SO_4 aqueous solution.

1.5 Photocurrent responsive measurements

The photoelectrochemical characterizations were performed on the electrochemical workstation (CHI 760e) with the assembled photoelectrodes as the working electrode, the Pt mesh as the counter electrode and the Ag/AgCl as the reference electrode. Meanwhile, the 0.2 M Na_2SO_4 aqueous solution was filled in the cell as the electrolyte. The light source and density were identical with that in the CO_2 photoreduction experiments.

1.6 Photocatalytic CO_2 reduction measurement

CO_2 photoreduction tests were performed on an evaluation system (CEL-SPH2NS9, AULTT, China), in a 100 mL quartz container, and irradiated with a 300 W Xe lamp, which intensity of light is 5.2×10^5 cd ($420 \leq \lambda \leq 800$ nm). A specific amount of catalysts were dispersed in 40 mL of MeCN aqueous solution, $[Ru(bpy)_3]Cl_2\cdot6H_2O$ (0.015 mmol) as a photosensitizer, TEOA (10 mL) as a sacrificial reagent, and transferred them into a glass container. Then, the container was saturated with high-purity CO_2 gas, repeated three times, and the reaction system temperature was ensured at 6 ℃ via a circulating water-cooling system outside the container. After reaction finished, the amounts of gaseous products (CO, CH_4 and H_2) were analyzed using a gas chromatography equipped with a flame ionization detector (FID), and a thermal conductivity detector (TCD).

1.7 Recycling experiments

Reusability and stability are important indicators to evaluate catalyst, after each reaction, the catalyst was recovered by centrifugation and washed several times with deionized water and then dried at 80 ℃ for 12 h before the next reaction.

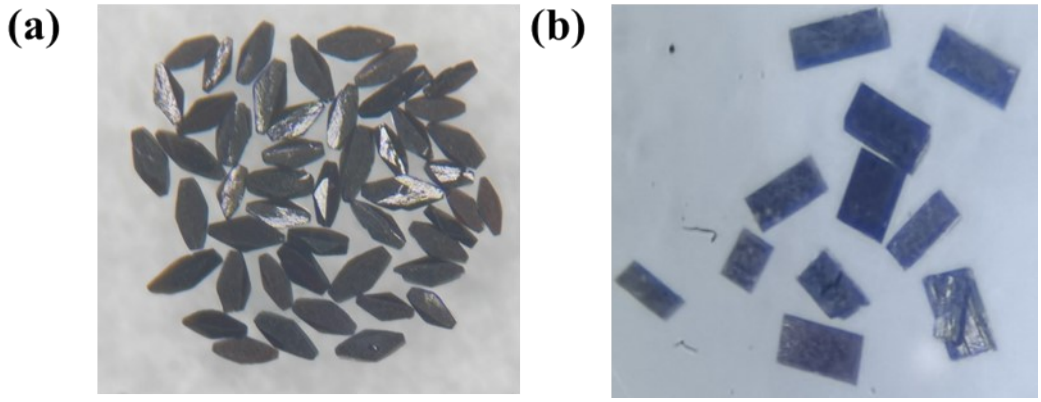

Fig. S1 The picture of crystal morphology for (a) compound **1** and (b) compound **2**.

2. Crystal structures

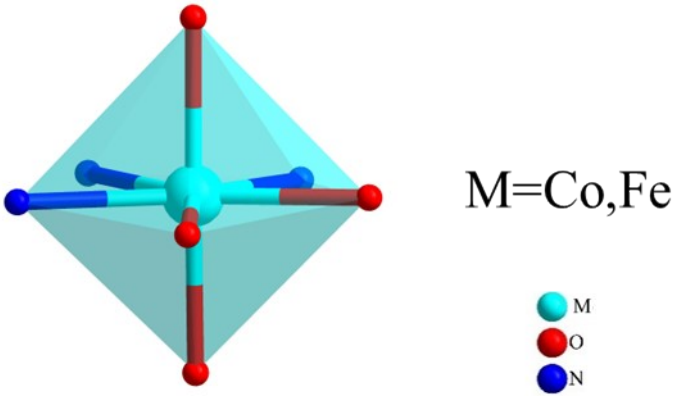

Fig. S2 Local coordination environments of {M} in compounds **1** and **2**.

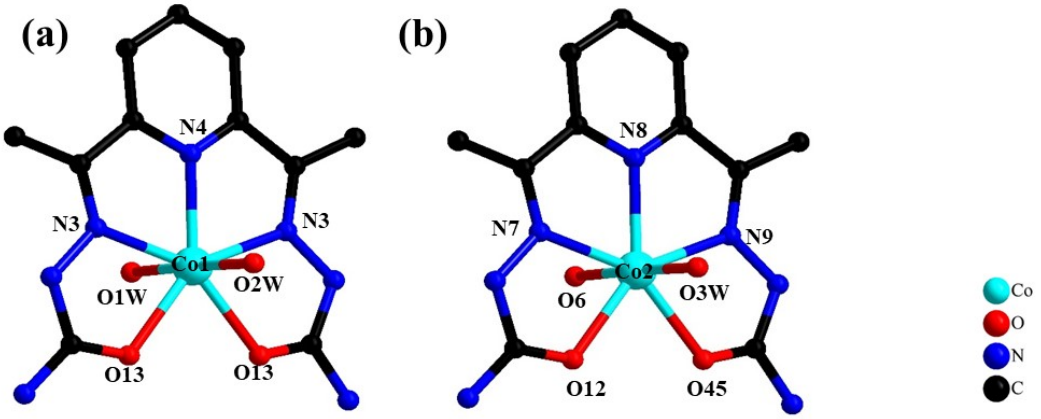

Fig. S3 Local coordination environments of DAPSC ligand with (a) Co1 and (b) Co2 in compound **1**.

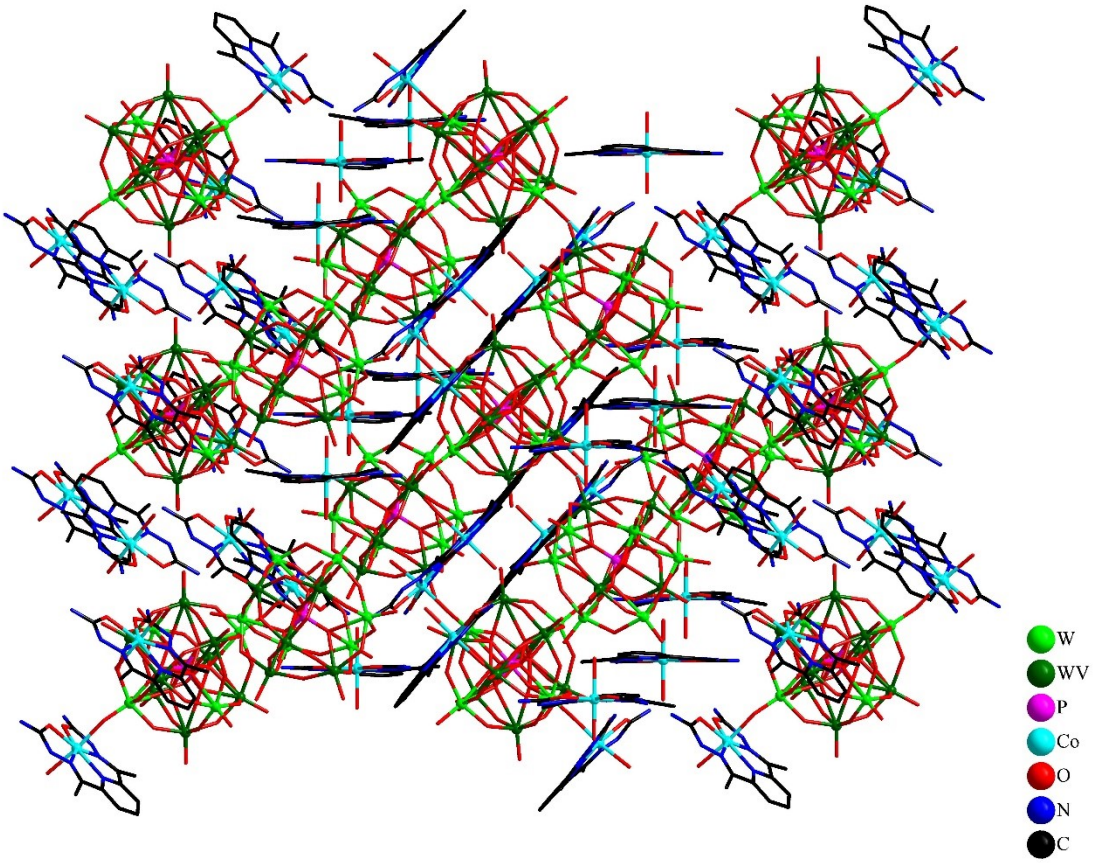

Fig. S4 The 3D supramolecular framework (ball-and-stick) of compound **1**.

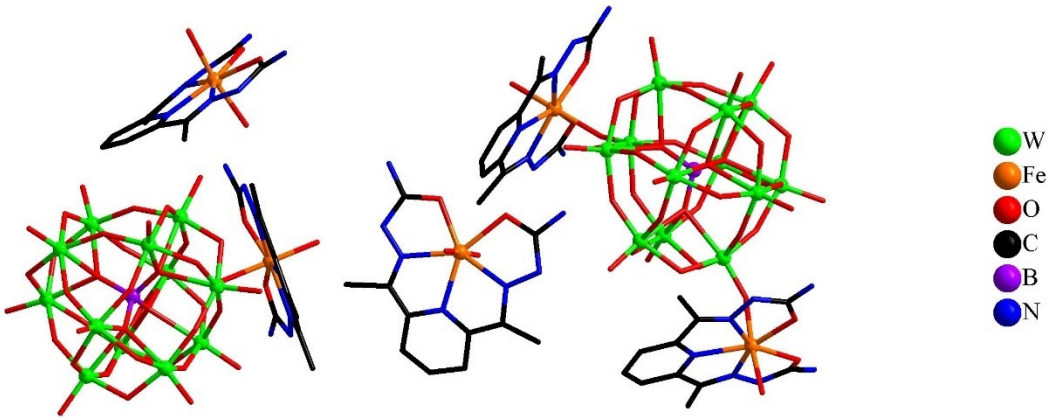

Fig. S5 The asymmetric unit of compound **2**.

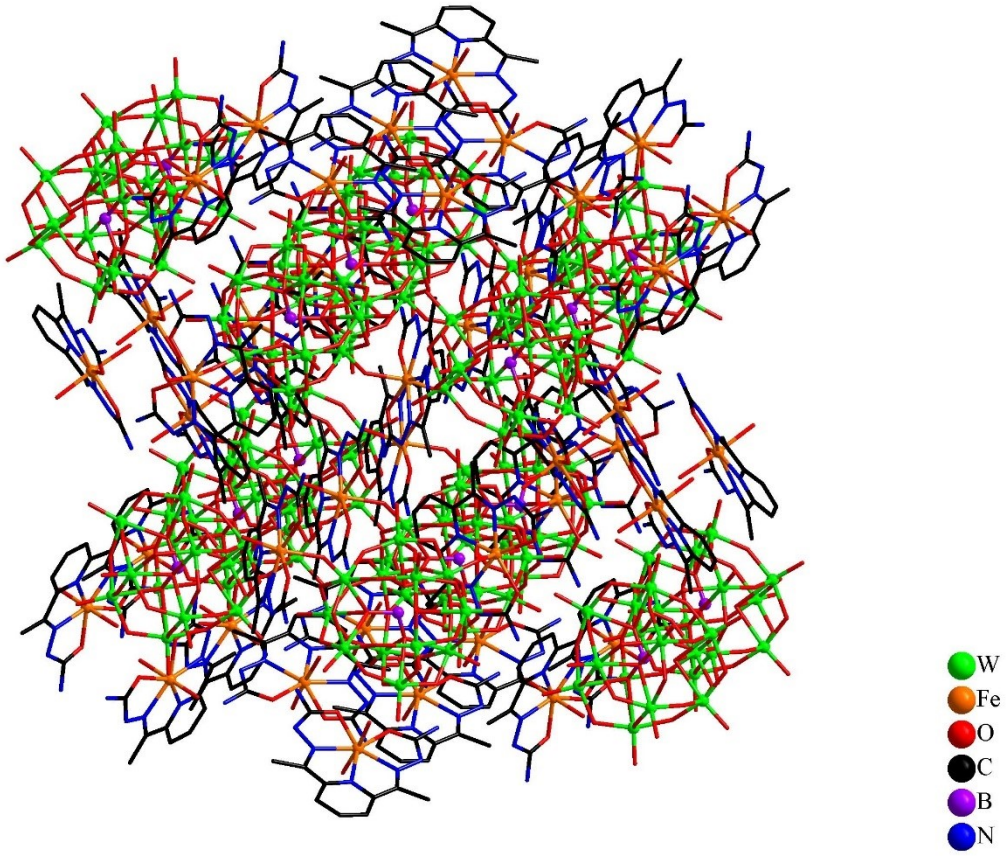

Fig. S6 The 3D supramolecular framework (ball-and-stick) of compound **2**.

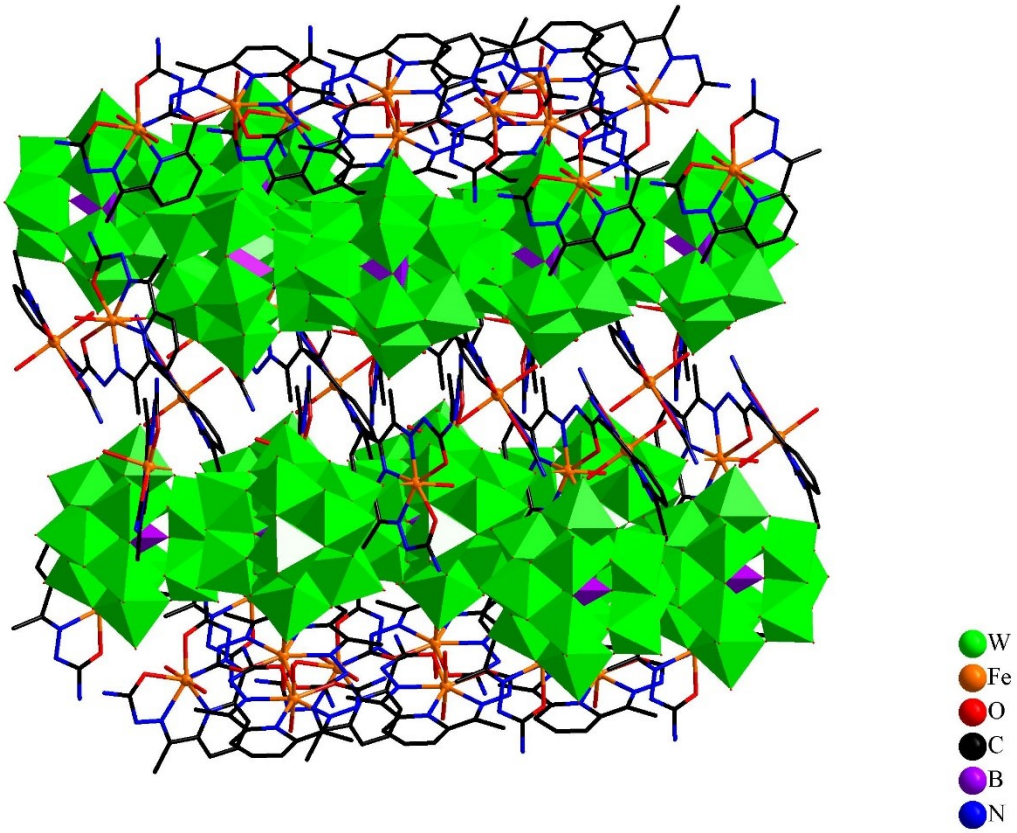

Fig. S7 The 3D supramolecular framework (polyhedral) of compound **2**.

3. Characterization

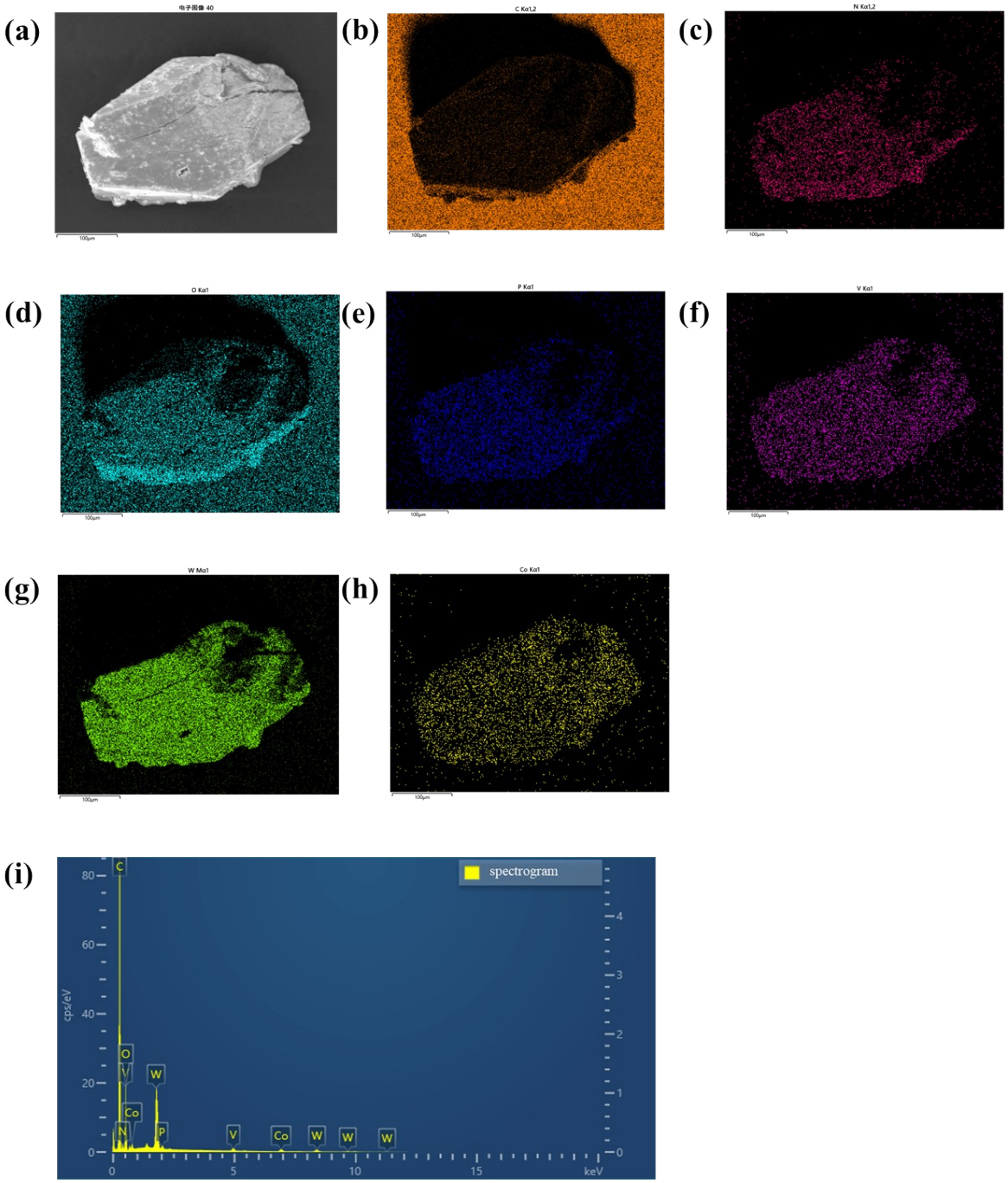

Fig. S8 The SEM image (a), the corresponding SEM-EDS elemental mapping of C, N, O, P, V, W, Co elements (b-h) and the map sum spectra (i) of compound **1**.

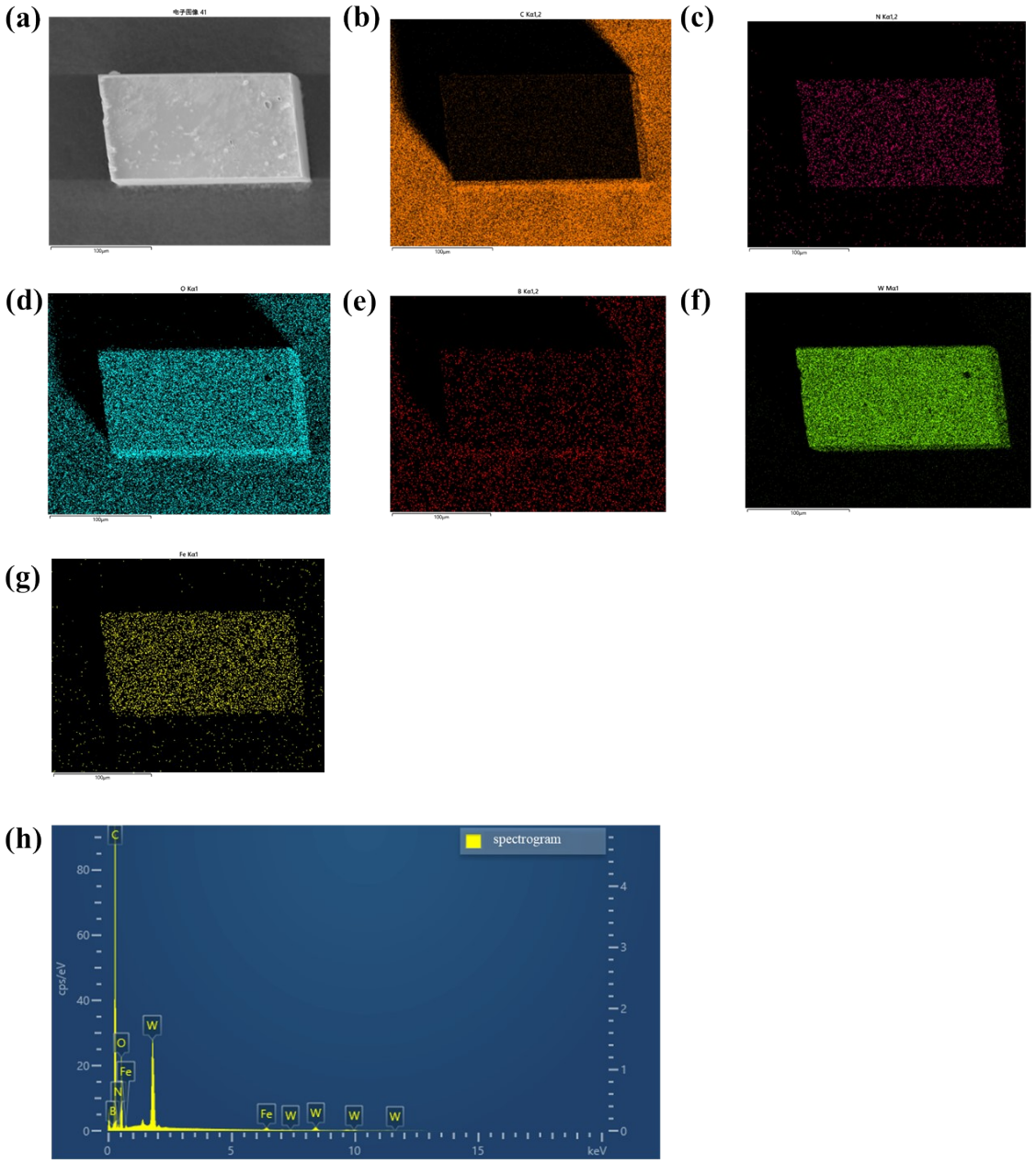

Fig. S9 The SEM image (a), the corresponding SEM-EDS elemental mapping of C, N, O, B, W, Fe elements (b-g) and the map sum spectra (h) of compound **2**.

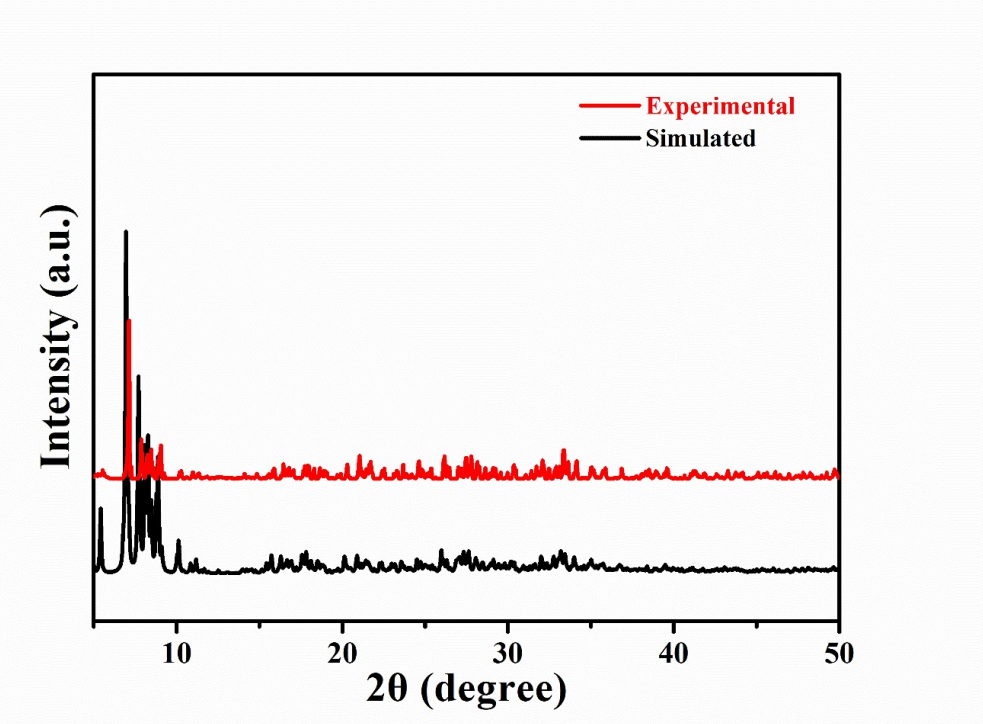

Fig. S10 The powder PXRD pattern of compound **1**.

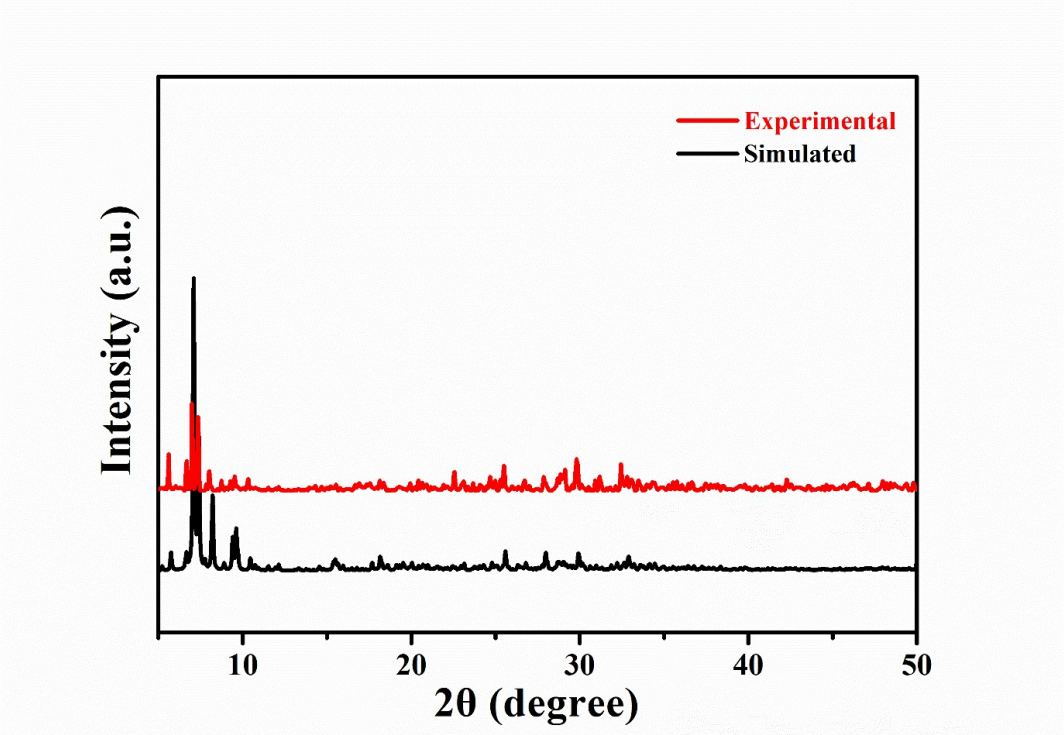

Fig. S11 The Powder PXRD pattern of compound **2**.

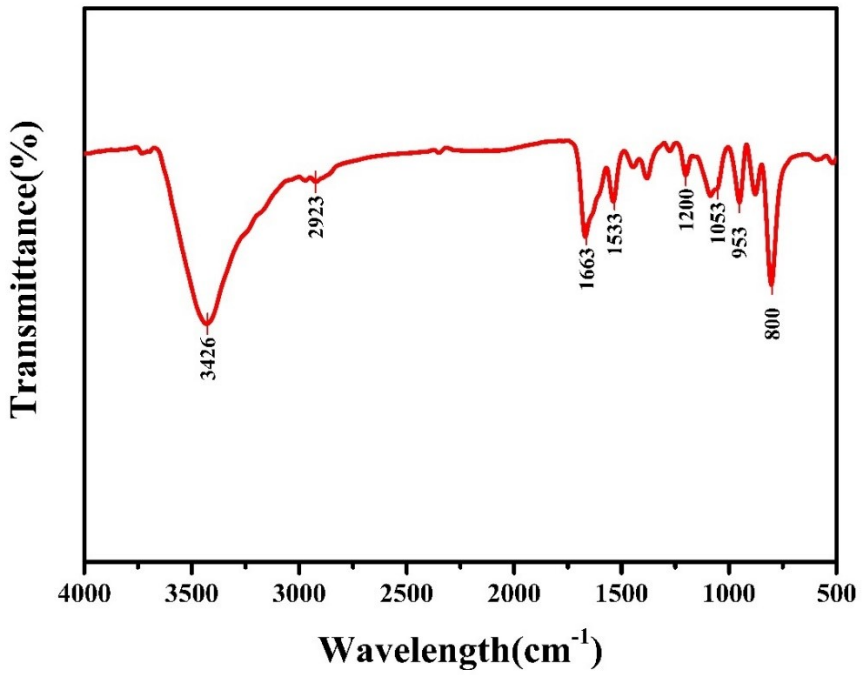

Fig. S12 The IR spectrum of compound **1**.

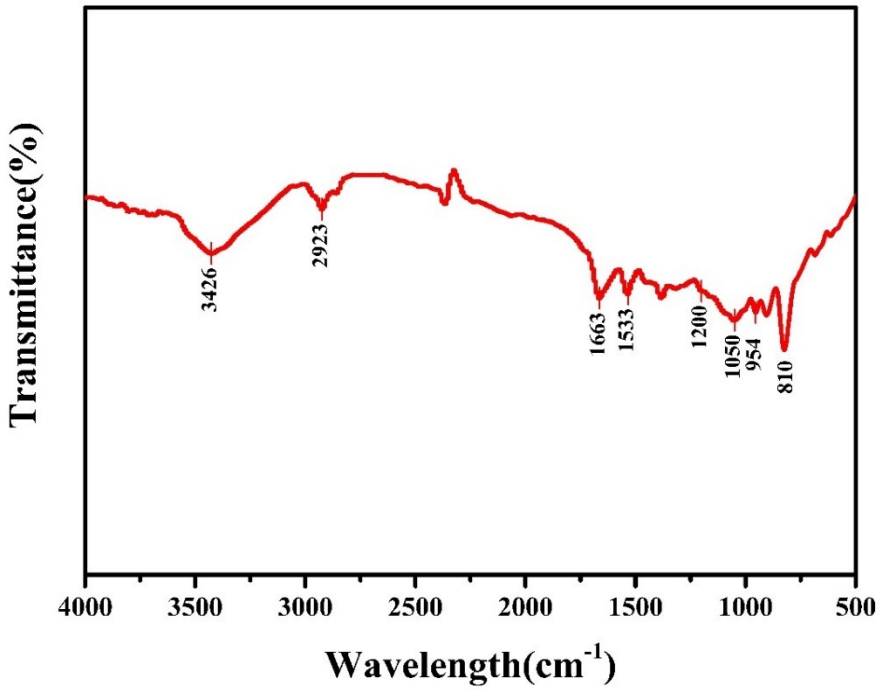

Fig. S13 The IR spectrum of compound **2**.

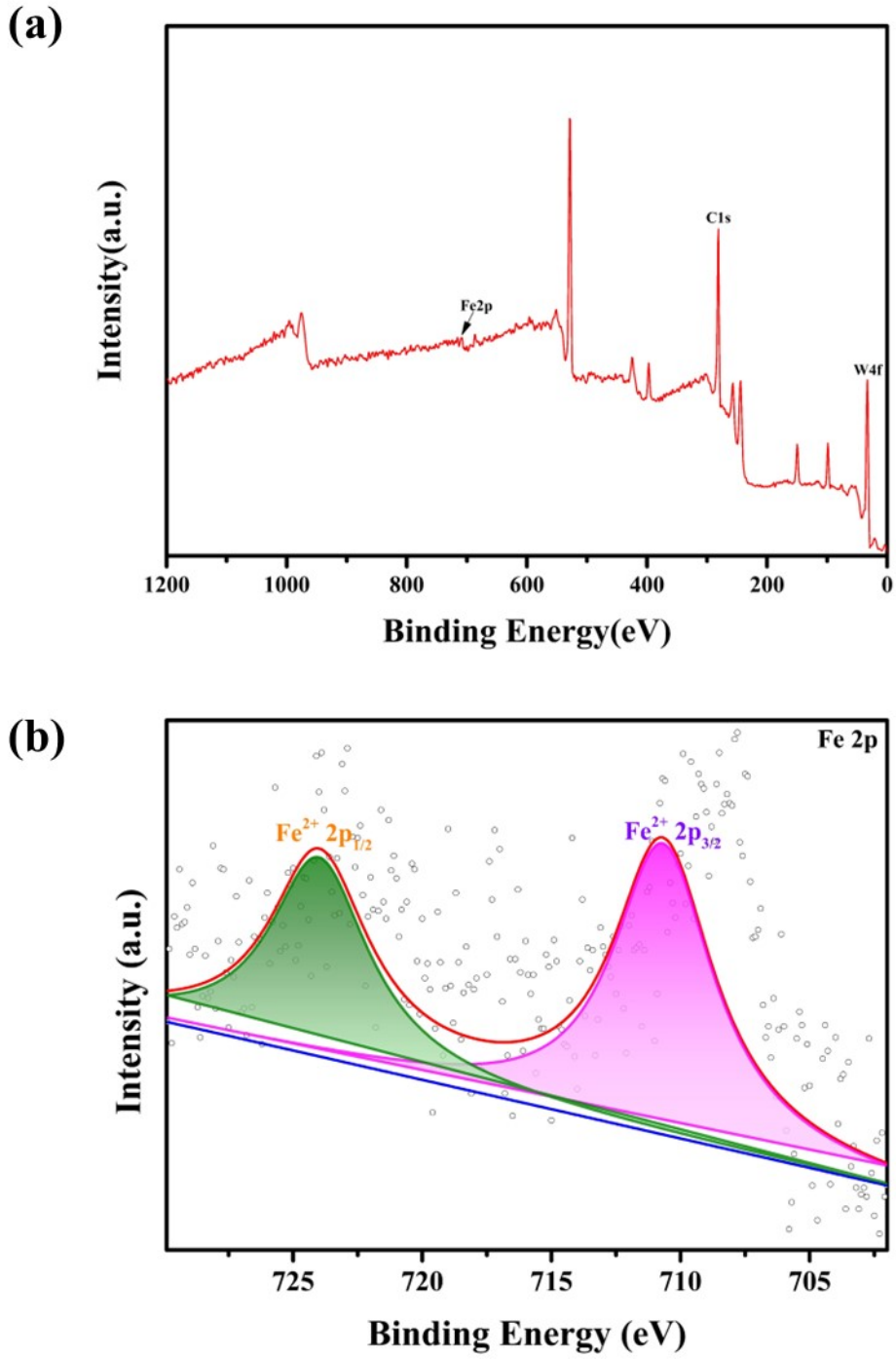

Fig. S14 (a) Full scan XPS spectrum, (b) Fe 2p high-resolution XPS spectrum of compound **2**.

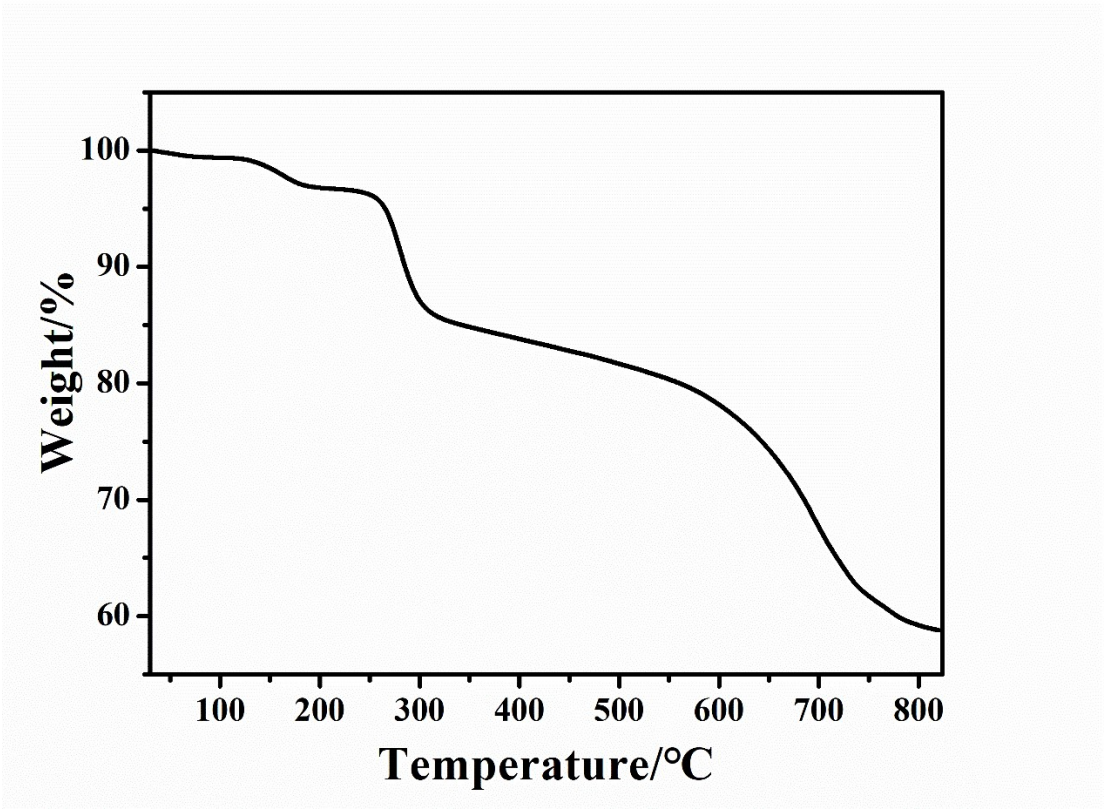

Fig. S15 Thermogravimetric analytical trace of compound **1**.

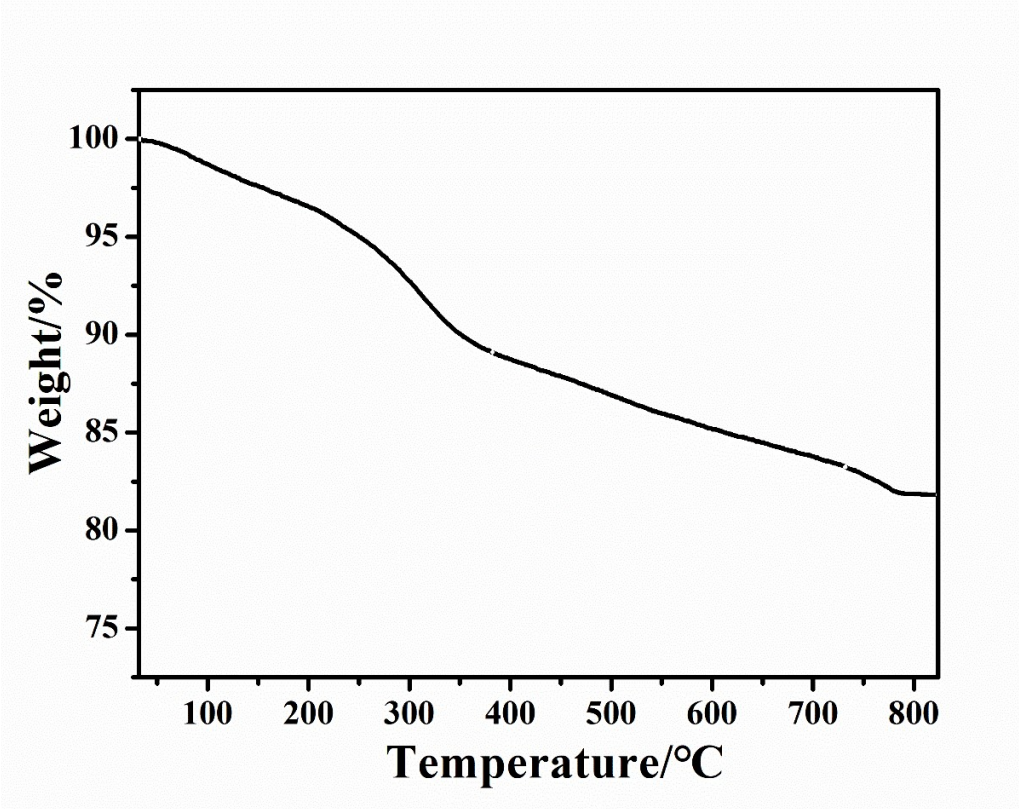

Fig. S16 Thermogravimetric analytical trace of compound **2**.

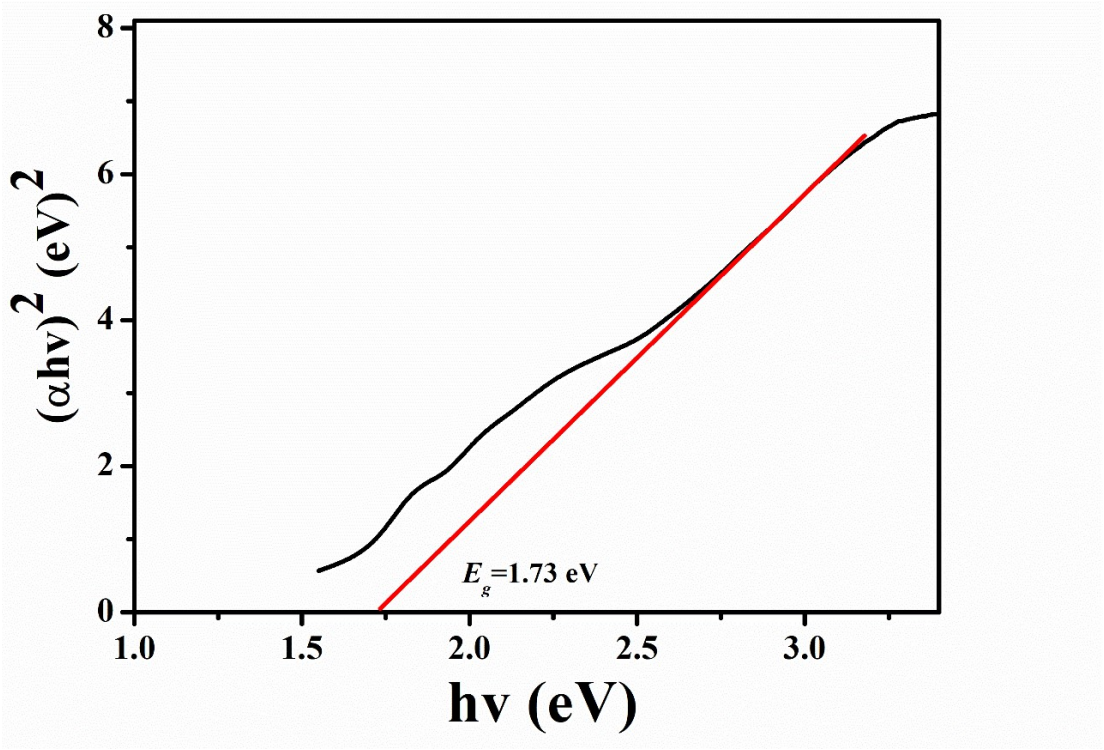

Fig. S17 Tauc plot for band-gap calculation of compound **2**.

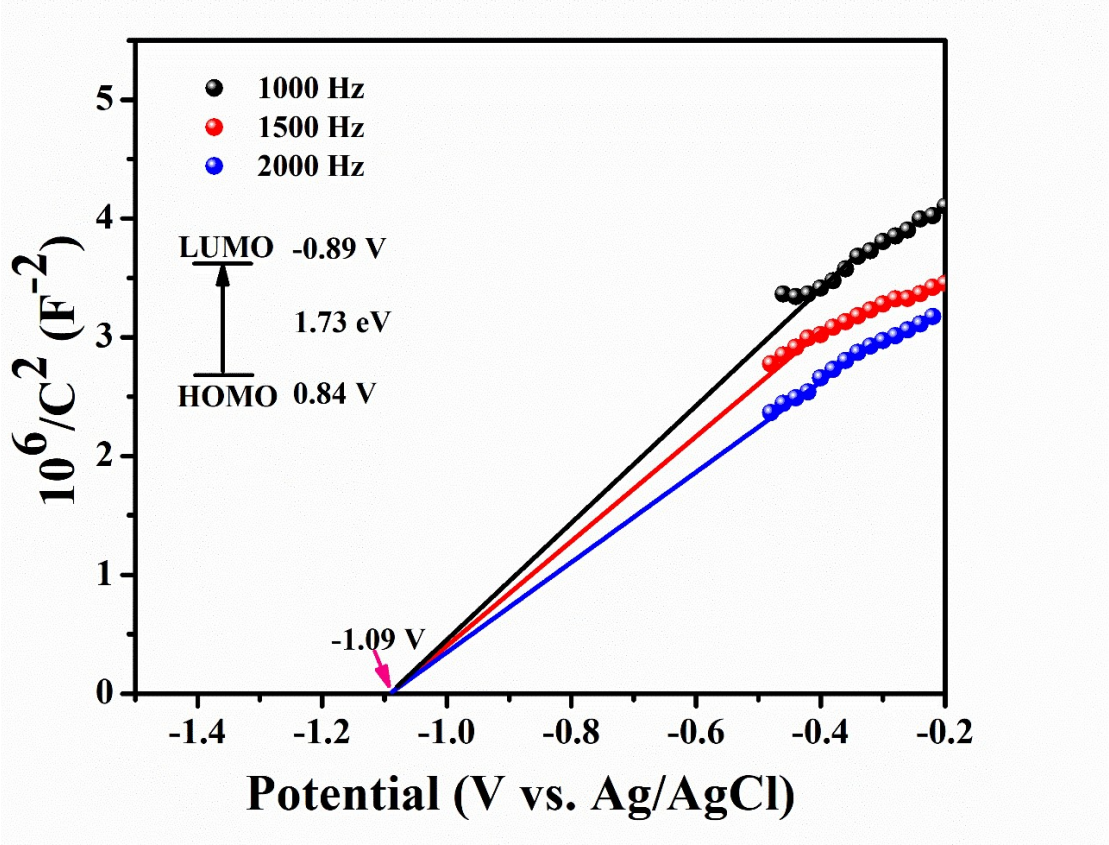

Fig. S18 Mott–Schottky plots for compound **2**.

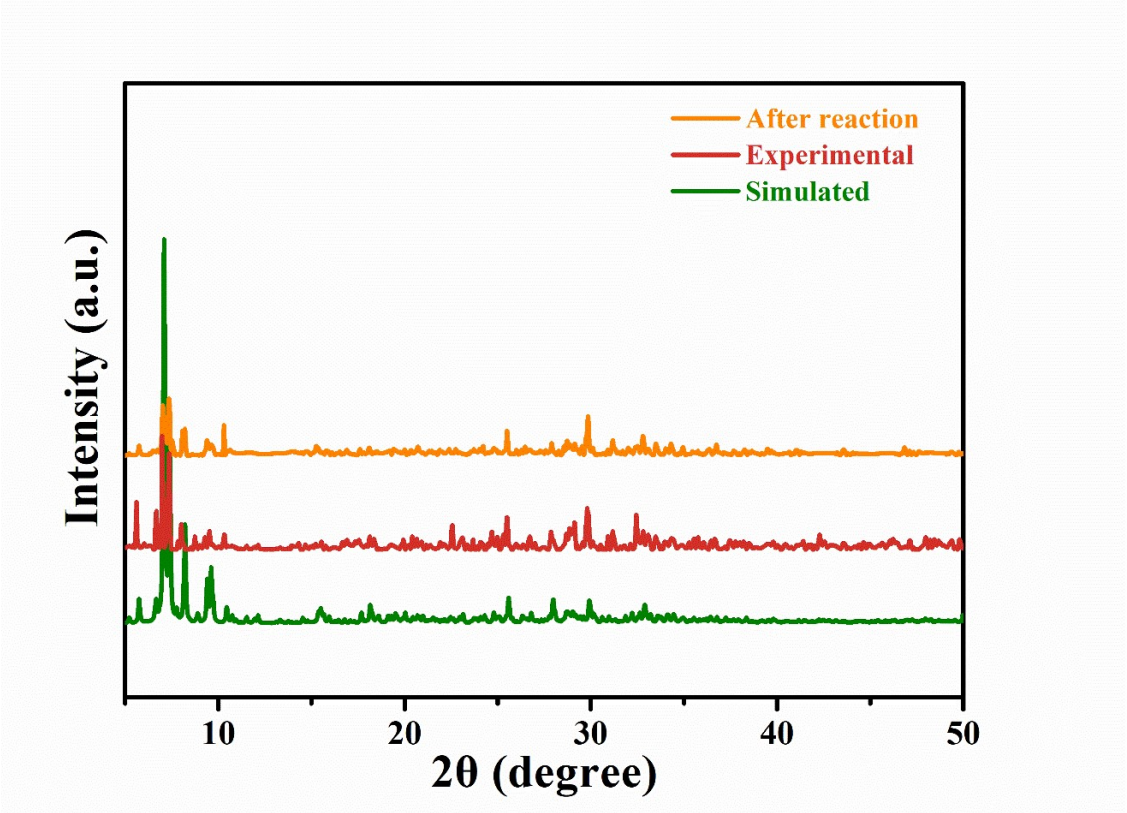

Fig. S19 PXRD patterns of compound **1** after the photocatalytic reaction.

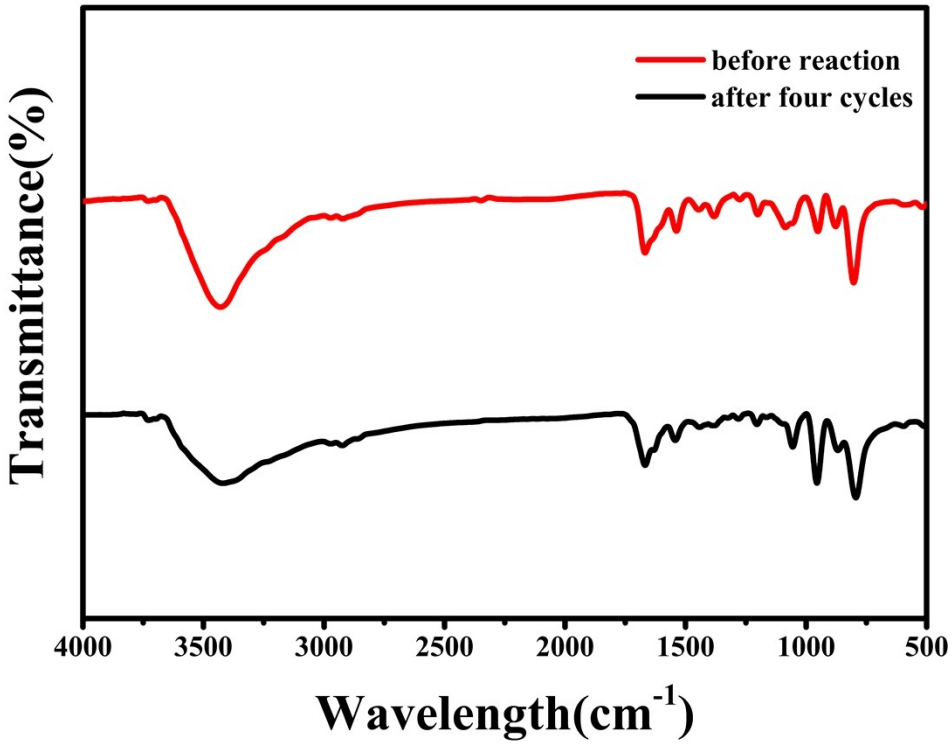

Fig. S20 IR patterns of compound **1** before reaction and after four cycles.

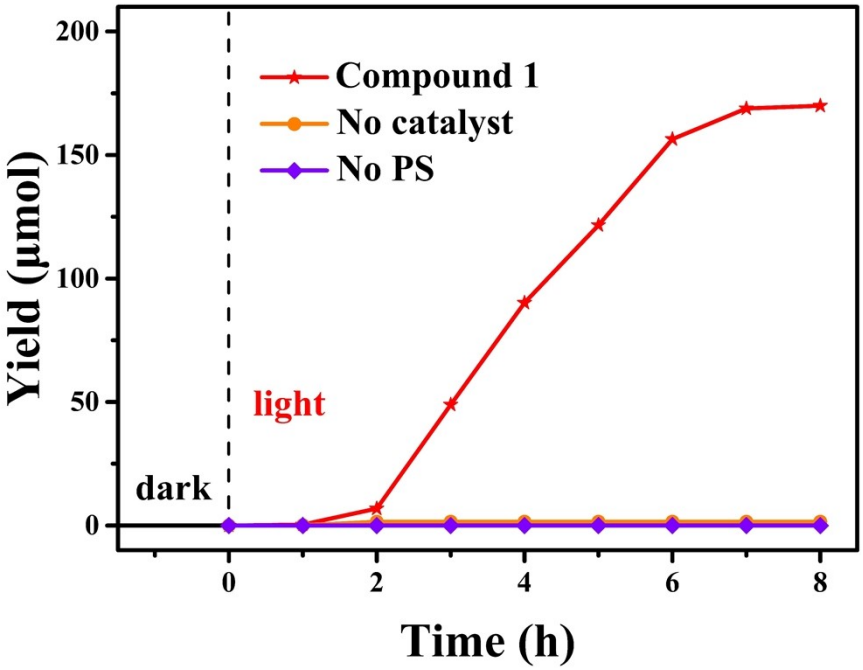

Fig. S21 Comparison of the yield of CO under different conditions.

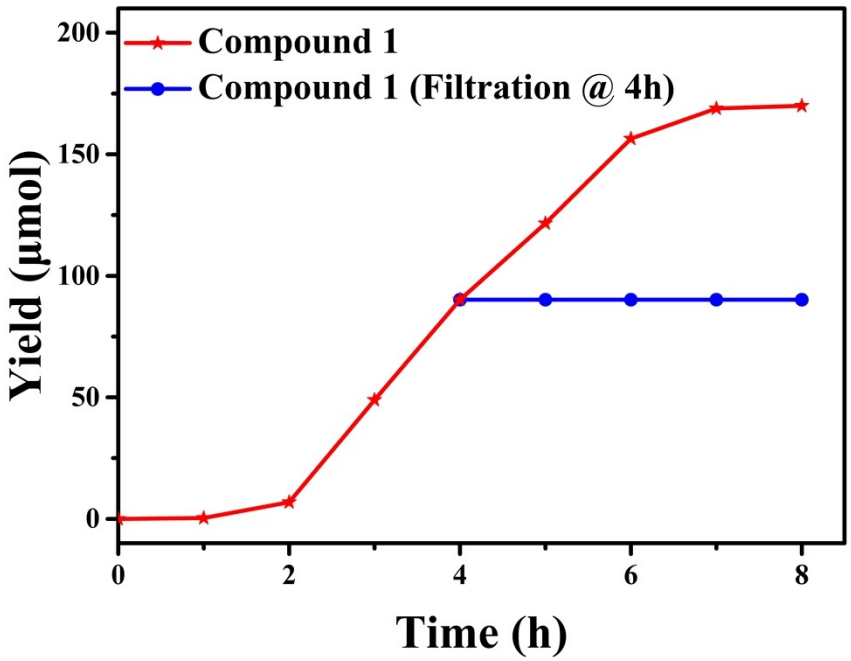

Fig. S22 Comparison of the yield of CO under different conditions.

Fig. S23 Photographs of the photocatalytic CO_2 reduction devices.

Table S1. Crystal data for compounds **1** and **2**.

Compound	**1**	**2**
Formula	$C_{66}H_{139}Co_6N_{42}O_{116.5}P_2V_2W_{22}$	$C_{55}H_{105}N_{28}Fe_5O_{109}B_2W_{24}$
Formula Weight	7947.28	7714.00
T (K)	293(2)	296(2)
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/m$	*P*-1
a (Å)	13.6935(4)	13.2589(7)
b (Å)	36.7469(8)	22.8458(11)
c (Å)	17.4310(4)	25.8955(13)
α (deg)	90	84.6220(10)
β (deg)	104.146(3)	80.1870(10)
γ (deg)	90	84.6560(10)
V (Å^3)	8505.2(4)	7671.4(7)
Z	2	2
D_c (mg m^{-3})	3.103	3.340
μ (mm^{-1})	15.612	18.479
F (000)	7254	6936
θ range (deg)	2.032-25.499	0.800-27.283
Crystal size (mm^3)	0.15 × 0.13 × 0.12	0.12 × 0.11 × 0.10
	-16≤h≤16	-16≤h≤16
Limiting indices	-44≤k≤44	-28≤k≤27
	-21≤l≤20	-33≤l≤32
Reflections/collected	85896	60830
Independent reflection/unique	16098	30423
R (int)	0.0868	0.0655
Data/restraints/parameters	16098/244/1233	30423/496/2080
GOF	1.142	1.029
R_1[a], wR_2 [I>2σ(I)]	R_1 = 0.0821,	R_1 = 0.0490,

	wR_2[b] = 0.1788	wR_2 = 0.1160
R_1, wR_2 (all data)	R_1 = 0.1005, wR_2 = 0.1856	R_1 = 0.0843, wR_2 = 0.1381

[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 S2. Selected bond lengths (Å) and bond angles (deg) for compound **1**

Co(1)-O(1W)	2.11(2)	N(4)-Co(1)-O(13)#2	142.8(3)
Co(1)-O(2W)	2.14(2)	O(13)-Co(1)-O(13)#2	74.5(7)
Co(1)-N(4)	2.17(2)	O(1W)-Co(1)-N(3)#2	89.7(5)
Co(1)-O(13)	2.180(14)	O(2W)-Co(1)-N(3)#2	90.5(5)
Co(1)-O(13)#2	2.180(14)	N(4)-Co(1)-N(3)#2	69.6(5)
Co(1)-N(3)#2	2.193(16)	O(13)-Co(1)-N(3)#2	147.6(6)
Co(1)-N(3)	2.193(16)	O(13)#2-Co(1)-N(3)#2	73.2(6)
Co(2)-O(12)	2.116(14)	O(1W)-Co(1)-N(3)	89.7(5)
Co(2)-O(3W)	2.133(18)	O(2W)-Co(1)-N(3)	90.5(5)
Co(2)-O(8)	2.153(13)	N(4)-Co(1)-N(3)	69.6(5)
Co(2)-O(45)	2.161(19)	O(13)-Co(1)-N(3)	73.2(6)
Co(2)-N(8)	2.167(19)	O(13)#2-Co(1)-N(3)	147.6(6)
Co(2)-N(7)	2.17(2)	N(3)#2-Co(1)-N(3)	139.2(9)
Co(2)-N(9)	2.175(18)	O(12)-Co(2)-O(3W)	84.5(7)
Co(3)-O(4W)	2.146(18)	O(12)-Co(2)-O(8)	89.7(6)
Co(3)-O(5W)	2.165(14)	O(3W)-Co(2)-O(8)	173.8(7)
Co(3)-N(15)	2.180(17)	O(12)-Co(2)-O(45)	76.2(6)
Co(3)-O(50)	2.184(16)	O(3W)-Co(2)-O(45)	88.4(9)
Co(3)-N(14)	2.186(18)	O(8)-Co(2)-O(45)	88.0(6)
Co(3)-O(24)	2.188(16)	O(12)-Co(2)-N(8)	143.3(7)
Co(3)-N(16A)	2.20(2)	O(3W)-Co(2)-N(8)	94.6(8)
Co(4)-N(14A)	2.155(18)	O(8)-Co(2)-N(8)	91.4(6)
Co(4)-N(14A)#2	2.155(18)	O(45)-Co(2)-N(8)	140.5(7)
Co(4)-O(6W)	2.16(2)	O(12)-Co(2)-N(7)	71.9(7)
Co(4)-N(15A)	2.17(3)	O(3W)-Co(2)-N(7)	93.2(9)
Co(4)-O(36)#2	2.181(16)	O(8)-Co(2)-N(7)	87.1(7)
Co(4)-O(36)	2.181(17)	O(45)-Co(2)-N(7)	147.7(7)
Co(4)-O(7W)	2.19(2)	N(8)-Co(2)-N(7)	71.5(7)
O(1W)-Co(1)-O(13)	89.6(7)	O(12)-Co(2)-N(9)	146.2(7)
O(2W)-Co(1)-O(13)	90.0(7)	O(3W)-Co(2)-N(9)	85.0(8)
N(4)-Co(1)-O(13)	142.8(3)	O(8)-Co(2)-N(9)	98.7(6)
O(1W)-Co(1)-O(13)#2	89.6(7)	O(45)-Co(2)-N(9)	71.5(7)
O(2W)-Co(1)-O(13)#2	90.0(7)	N(8)-Co(2)-N(9)	69.6(7)
N(7)-Co(2)-N(9)	140.7(8)	N(14A)-Co(4)-O(6W)	87.8(5)
O(4W)-Co(3)-O(5W)	178.4(7)	N(14A)#2-Co(4)-O(6W)	87.8(5)
O(4W)-Co(3)-N(15)	89.6(7)	N(14A)-Co(4)-N(15A)	71.3(5)

O(5W)-Co(3)-N(15)	92.0(6)	N(14A)#2-Co(4)-N(15A)	71.3(5)
O(4W)-Co(3)-O(50)	91.5(8)	O(6W)-Co(4)-N(15A)	91.2(9)
O(5W)-Co(3)-O(50)	87.5(7)	N(14A)-Co(4)-O(36)#2	146.0(7)
N(15)-Co(3)-O(50)	141.6(7)	N(14A)#2-Co(4)-O(36)#2	71.6(7)
O(4W)-Co(3)-N(14)	91.4(8)	O(6W)-Co(4)-O(36)#2	90.7(7)
O(5W)-Co(3)-N(14)	88.8(6)	N(15A)-Co(4)-O(36)#2	142.7(4)
N(15)-Co(3)-N(14)	71.1(7)	N(14A)-Co(4)-O(36)	71.6(7)
O(50)-Co(3)-N(14)	147.2(6)	N(14A)#2-Co(4)-O(36)	146.0(7)
O(4W)-Co(3)-O(24)	87.4(7)	O(6W)-Co(4)-O(36)	90.7(7)
O(5W)-Co(3)-O(24)	91.1(6)	N(15A)-Co(4)-O(36)	142.7(4)
N(15)-Co(3)-O(24)	142.8(7)	O(36)#2-Co(4)-O(36)	74.4(8)
O(50)-Co(3)-O(24)	75.6(6)	N(14A)-Co(4)-O(7W)	92.4(6)
N(14)-Co(3)-O(24)	71.9(6)	N(14A)#2-Co(4)-O(7W)	92.4(6)
O(4W)-Co(3)-N(16A)	86.6(8)	O(6W)-Co(4)-O(7W)	179.5(9)
O(5W)-Co(3)-N(16A)	94.2(7)	N(15A)-Co(4)-O(7W)	89.3(10)
N(15)-Co(3)-N(16A)	70.9(8)	O(36)#2-Co(4)-O(7W)	88.9(8)
O(50)-Co(3)-N(16A)	70.8(8)	O(36)-Co(4)-O(7W)	88.9(8)
N(14)-Co(3)-N(16A)	141.9(8)	N(14A)#2-Co(4)-O(36)#2	71.6(7)
O(24)-Co(3)-N(16A)	145.7(8)	N(14A)-Co(4)-N(14A)#2	142.2(11)

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

Table S3. Selected bond lengths (Å) and bond angles (deg) for compound **2**.

Fe(1)-O(3W)	2.155(15)	O(2A)-Fe(1)-N(02P)	140.3(6)
Fe(1)-O(4W)	2.189(16)	O(3W)-Fe(1)-N(03I)	92.0(6)
Fe(1)-O(2A)	2.204(13)	O(4W)-Fe(1)-N(03I)	94.6(6)
Fe(1)-N(02P)	2.190(17)	O(2A)-Fe(1)-N(03I)	149.6(6)
Fe(1)-N(03I)	2.210(16)	N(02P)-Fe(1)-N(03I)	70.0(6)
Fe(1)-O(1A)	2.205(15)	O(3W)-Fe(1)-O(1A)	85.8(7)
Fe(1)-N(03F)	2.249(17)	O(4W)-Fe(1)-O(1A)	91.0(7)
Fe(2)-O(1W)	2.110(17)	O(2A)-Fe(1)-O(1A)	79.2(6)
Fe(2)-O(67)	2.165(16)	N(02P)-Fe(1)-O(1A)	140.4(6)
Fe(2)-N(02N)	2.21(2)	N(03I)-Fe(1)-O(1A)	70.5(6)
Fe(2)-O(69)	2.209(16)	O(3W)-Fe(1)-N(03F)	93.2(7)
Fe(2)-O(61)	2.213(16)	O(4W)-Fe(1)-N(03F)	85.5(6)
Fe(2)-N(02Z)	2.230(17)	O(2A)-Fe(1)-N(03F)	70.9(6)
Fe(2)-N(02W)	2.244(19)	O(4W)-Fe(1)-O(1A)	91.0(7)
Fe(3)-O(60)	2.156(16)	O(2A)-Fe(1)-O(1A)	79.2(6)
Fe(3)-O(58)	2.206(14)	N(02P)-Fe(1)-O(1A)	140.4(6)
Fe(3)-N(03Z)	2.17(2)	N(03I)-Fe(1)-O(1A)	70.5(6)
Fe(3)-N(03C)	2.208(18)	O(3W)-Fe(1)-N(03F)	93.2(7)
Fe(3)-N(031)	2.219(18)	O(4W)-Fe(1)-N(03F)	85.5(6)
Fe(3)-O(2W)	2.231(15)	O(2A)-Fe(1)-N(03F)	70.9(6)
Fe(3)-O(76)	2.286(15)	N(02P)-Fe(1)-N(03F)	69.4(6)
Fe(4)-O(5W)	1.919(19)	N(03I)-Fe(1)-N(03F)	139.4(6)

Fe(4)-O(4A)	2.085(18)	O(1A)-Fe(1)-N(03F)	150.1(6)
Fe(4)-O(6W)	2.113(17)	O(1W)-Fe(2)-O(67)	166.8(7)
Fe(4)-O(3A)	2.157(16)	O(1W)-Fe(2)-N(02N)	83.6(7)
Fe(4)-N(03G)	2.18(2)	O(67)-Fe(2)-N(02N)	92.9(6)
Fe(4)-N(03U)	2.181(18)	O(1W)-Fe(2)-O(69)	87.2(7)
Fe(4)-N(03V)	2.170(18)	O(67)-Fe(2)-O(69)	89.8(6)
O(3W)-Fe(1)-O(4W)	171.2(6)	N(02N)-Fe(2)-O(69)	151.1(7)
O(3W)-Fe(1)-O(2A)	86.5(6)	O(1W)-Fe(2)-O(61)	83.1(7)
O(4W)-Fe(1)-O(2A)	84.8(6)	O(67)-Fe(2)-O(61)	83.7(6)
O(3W)-Fe(1)-N(02P)	96.3(7)	N(02N)-Fe(2)-O(61)	71.5(6)
O(4W)-Fe(1)-N(02P)	91.4(7)	O(69)-Fe(2)-O(61)	80.3(7)
O(1W)-Fe(2)-N(02Z)	94.7(8)	O(5W)-Fe(4)-O(3A)	94.1(7)
O(67)-Fe(2)-N(02Z)	95.9(6)	O(4A)-Fe(4)-O(3A)	75.1(6)
N(02N)-Fe(2)-N(02Z)	68.7(7)	O(6W)-Fe(4)-O(3A)	86.1(7)
O(69)-Fe(2)-N(02Z)	139.6(7)	O(5W)-Fe(4)-N(03G)	94.9(8)
O(61)-Fe(2)-N(02Z)	140.1(7)	O(4A)-Fe(4)-N(03G)	141.7(7)
O(1W)-Fe(2)-N(02W)	99.2(7)	O(6W)-Fe(4)-N(03G)	84.8(7)
O(67)-Fe(2)-N(02W)	92.0(7)	O(3A)-Fe(4)-N(03G)	140.4(7)
N(02N)-Fe(2)-N(02W)	137.4(7)	O(5W)-Fe(4)-N(03U)	92.5(8)
O(69)-Fe(2)-N(02W)	71.1(7)	O(4A)-Fe(4)-N(03U)	71.5(7)
O(61)-Fe(2)-N(02W)	151.1(6)	O(6W)-Fe(4)-N(03U)	87.4(7)
N(02Z)-Fe(2)-N(02W)	68.7(7)	O(3A)-Fe(4)-N(03U)	146.4(7)
O(60)-Fe(3)-O(58)	86.5(6)	N(03G)-Fe(4)-N(03U)	71.3(7)
O(60)-Fe(3)-N(03Z)	71.4(7)	O(5W)-Fe(4)-N(03V)	92.2(8)
O(58)-Fe(3)-N(03Z)	91.1(6)	O(4A)-Fe(4)-N(03V)	145.6(7)
O(60)-Fe(3)-N(03C)	147.3(7)	O(6W)-Fe(4)-N(03V)	87.6(7)
O(58)-Fe(3)-N(03C)	87.3(6)	O(3A)-Fe(4)-N(03V)	71.0(7)
N(03Z)-Fe(3)-N(03C)	140.8(7)	N(03G)-Fe(4)-N(03V)	70.2(7)
O(60)-Fe(3)-N(031)	141.8(7)	N(031)-Fe(3)-O(76)	140.1(6)
O(58)-Fe(3)-N(031)	93.4(6)	O(2W)-Fe(3)-O(76)	90.5(6)
N(03Z)-Fe(3)-N(031)	70.4(7)	O(5W)-Fe(4)-O(4A)	95.8(8)
N(03C)-Fe(3)-N(031)	70.6(7)	O(5W)-Fe(4)-O(6W)	179.7(8)
O(60)-Fe(3)-O(2W)	87.2(6)	O(4A)-Fe(4)-O(6W)	84.5(7)
O(58)-Fe(3)-O(2W)	173.6(6)	N(03U)-Fe(4)-N(03V)	141.5(7)
N(03Z)-Fe(3)-O(2W)	87.6(6)	O(58)-Fe(3)-O(76)	87.5(6)
N(03C)-Fe(3)-O(2W)	97.7(6)	N(03Z)-Fe(3)-O(76)	149.5(7)
N(031)-Fe(3)-O(2W)	92.0(6)	N(03C)-Fe(3)-O(76)	69.6(6)
O(60)-Fe(3)-O(76)	78.1(6)		

Table S4. The BVS calculation result of W atoms in $[PW^{VI}_{9}W^{V}_{2}V^{IV}O_{40}]^{7-}$ of compound 1.

W1	O2	1.672	BVS = 6.22	W8	O32	1.683	BVS = 6.29
	O3	1.892			O17	1.873	
	O16	1.904			O7	1.893	
	O10	1.908			O25	1.907	
	O4	1.925			O22	1.910	
	O18	2.424			O6	2.454	
W2	O20	1.691	BVS = 6.06	W9	O19	1.671	BVS = 6.30
	O17	1.883			O1	1.873	
	O14	1.900			O9	1.896	
	O23	1.912			O10	1.914	
	O11	1.940			O15	1.934	
	O5	2.440			O18	2.400	
W3	O33	1.708	BVS = 6.07	W11	O34	1.71	BVS = 6.01
	O7	1.874			O25	1.895	
	O23	1.896			O25#2	1.895	
	O15	1.899			O9	1.911	
	O16	1.925			O9#2	1.911	
	O18	2.440			O6	2.403	
W5	O21	1.652	BVS = 6.48				
	O4#2	1.897					
	O4	1.897					
	O11#2	1.910					
	O11	1.910					
	O5	2.36					

The calculated value of average oxidation state of W: 6.20

Table S5. The BVS calculation result of W atoms in $[PW^{VI}_{11}V^{IV}O_{40}]^{5-}$ of compound 1.

W4	O8	1.690	BVS = 6.29	W10	O49	1.656	BVS = 6.78
	O48	1.877			O51#1	1.865	
	O37#1	1.88			O26	1.866	
	O51	1.898			O38#1	1.900	
	O43	1.909			O27	1.922	
	O29	2.48			O28	2.37	
					O31	2.51	
W6	O46	1.700	BVS = 6.43	W12	O41	1.685	BVS = 6.59
	O52	1.877			O42	1.854	
	O26	1.881			O39	1.874	
	O42	1.890			O27	1.887	
	O44	1.910			O43	1.901	
	O30	2.40			O29	2.34	
	O31	2.43					
W7	O35	1.675	BVS = 6.72	W13	O40	1.652	BVS = 6.91
	O38	1.858			O37	1.87	
	O47	1.867			O39#1	1.87	
	O44	1.877			O52	1.87	
	O48	1.933			O47	1.877	
	O28#1	2.37			O29#1	2.41	
	O30	2.45					

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

The calculated value of average oxidation state of W: 6.62

4. Reference

1. A. A. A. Abu-Hussen and W. Linert, *Spectrochim. Acta. A Mol. Biomol. Spectrosc.*, 2009, **74**, 214-223.