Electronic Supplementary Information (ESI†)

A new 3D POMOF with two channels consisting of Wells-Dawson arsenotungstate and $\{Cl_4Cu_{10}(pz)_{11}\}$ complexes: synthesis, crystal structure, and properties

Bo-Wen Cong,[a] Zhan-Hua Su*,[a] Zhi-Feng Zhao*[b] Wen-Qi Zhao,[a] Xiu-Juan Ma,[a] Qiu Xu [a] and Li-Juan Du[a]

[a]*Key Laboratory of Photochemical Biomaterials and Energy Storage Materials, Heilongjiang Province, College of Chemistry and Chemical Engineering, Harbin Normal University, Harbin 150025, China*
[b]*College of Material Science and Engineering, Heilongjiang University of Science and Technology, Harbin 150022, China.*

Table of contents:

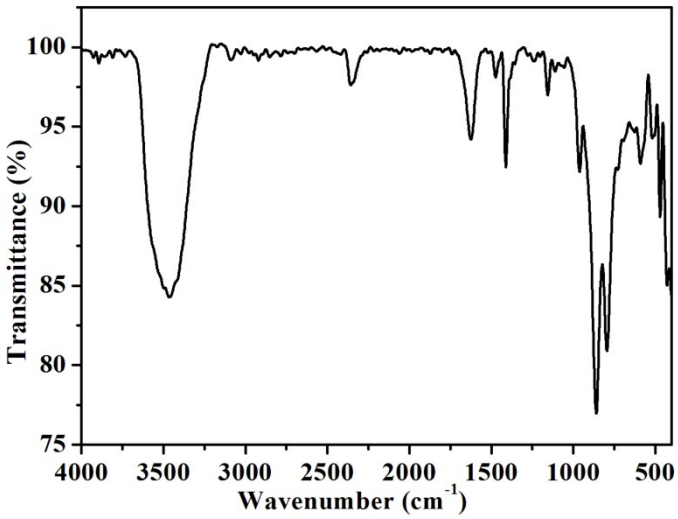

Fig. S1 IR spectrum of compound **1**.

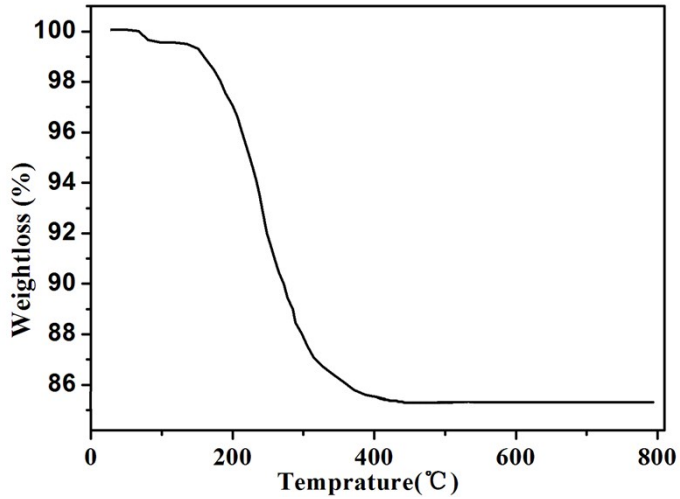

Fig. S2 The TG curve of compound **1**.

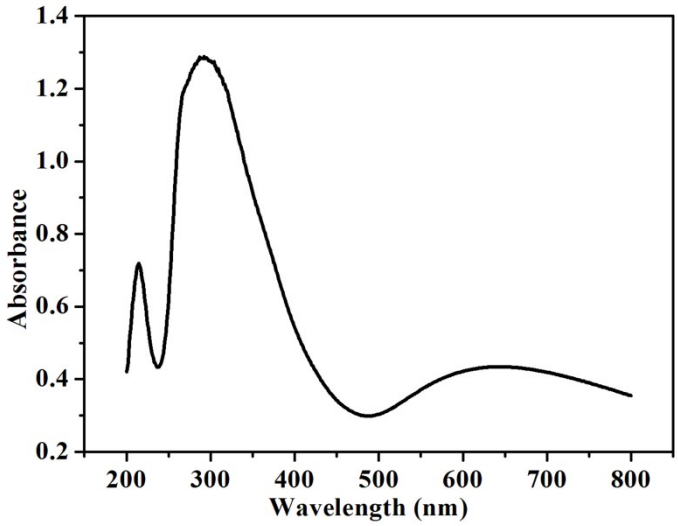

Fig. S3 The UV-vis spectrum of compound **1** in solid state at room temperature.

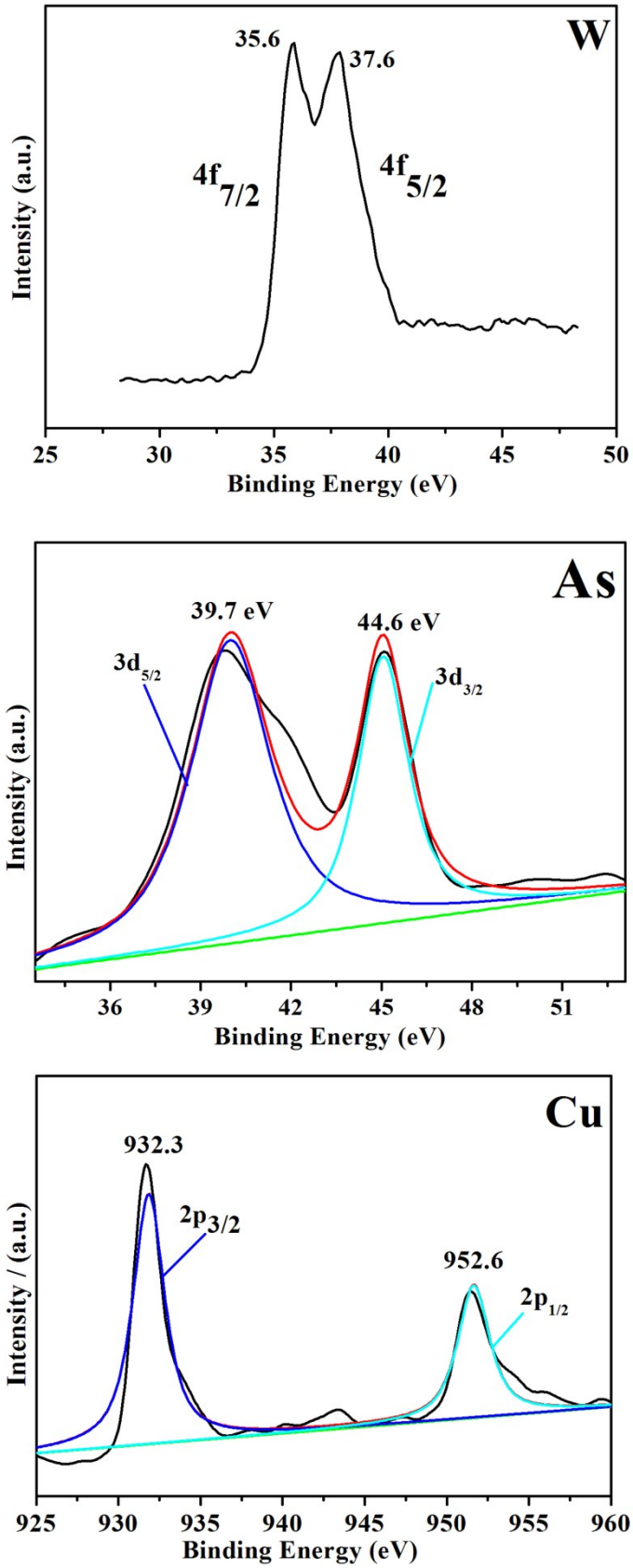

Fig. S4 The XPS spectra of compound **1**.

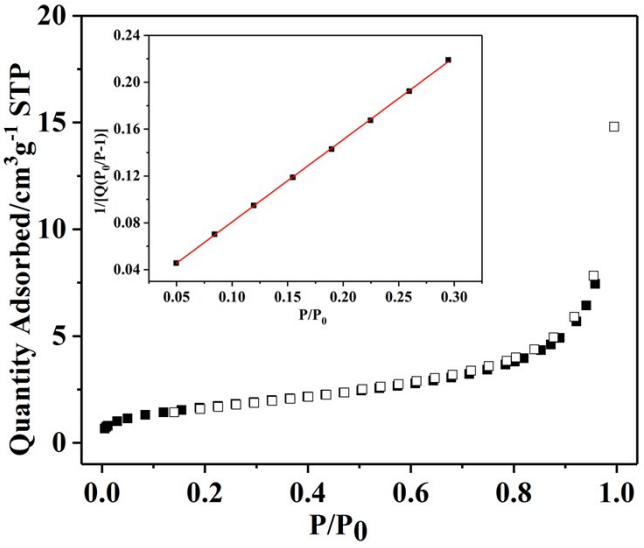

Fig. S5 N_2 sorption isotherm of compound **1** at 77 K (P_0 = 1 atm).

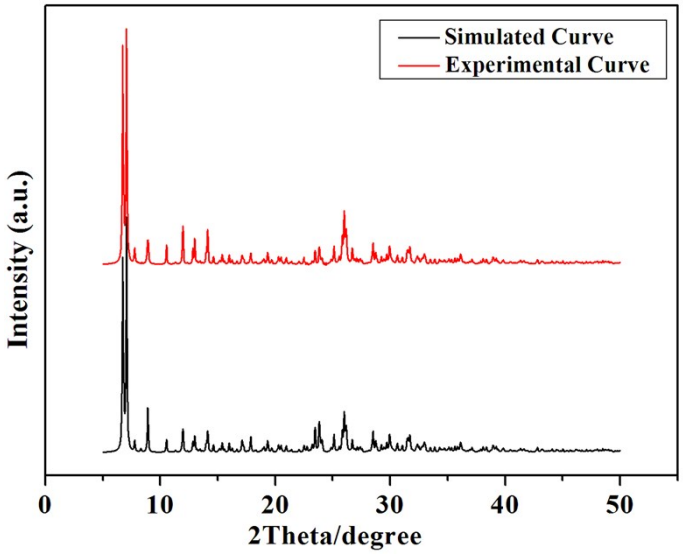

Fig. S6 The PXRD contrast curves of compound **1**.

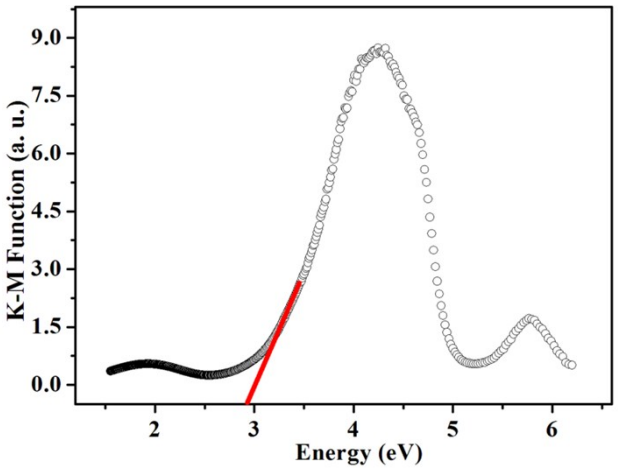

Fig. S7 Diffuse reflection spectrum of *Kubelka-Munk* (K-M) function versus energy (eV) of compound **1**.

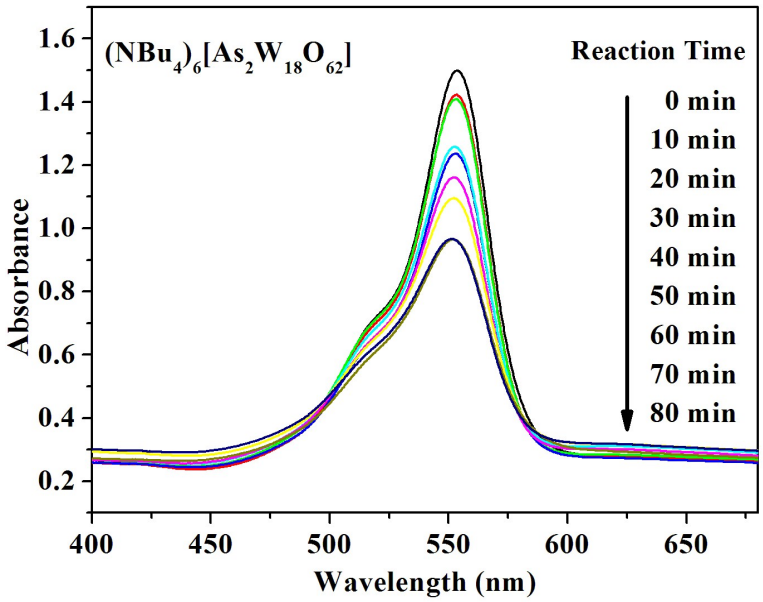

Fig. S8 Absorption spectra of the RhB aqueous solution during the photodegradation with $(NBu_4)_6[As_2W_{18}O_{62}]$ power

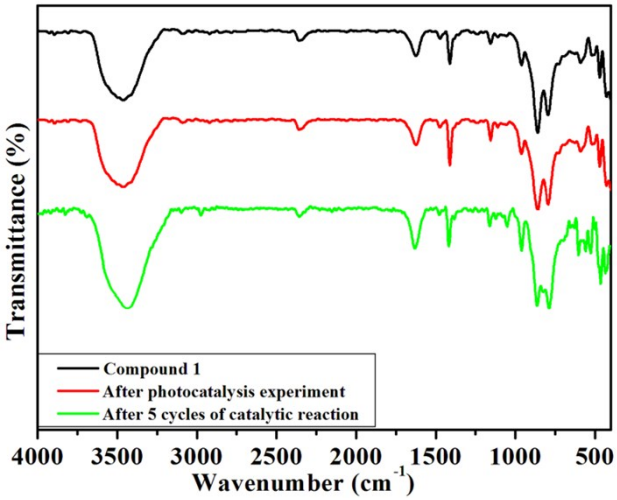

Fig. S9 The IR spectra of compound **1** before and after cycle reaction.

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

Compound **1**					
W(1)-O(9)	1.865(7)	W(1)-O(2)	1.890(7)	W(1)-O(4)	1.940(7)
W(1)-O(7)	1.972(8)	W(1)-O(1)	2.337(7)	W(1)-O(31)	1.690(8)
W(2)-O(1)	2.372(7)	W(2)-O(2)	1.956(8)	W(2)-O(3)	1.925(7)
W(2)-O(29)	1.919(7)	W(2)-O(14)	1.838(8)	W(2)-O(30)	1.711(7)
W(3)-O(1)	2.398(6)	W(3)-O(5)	1.941(7)	W(3)-O(4)	1.901(7)
W(3)-O(16)	1.885(8)	W(3)-O(28)	1.704(7)	W(3)-O(3)	1.907(8)
W(4)-O(27)	1.709(8)	W(4)-O(26)	1.884(7)	W(4)-O(6)	1.898(6)

W(4)-O(18)	1.925(7)	W(4)-O(5)	2.026(8)	W(4)-O(17)	2.315(7)
W(5)-O(25)	1.715(8)	W(5)-O(6)	1.891(6)	W(5)-O(26)#1	1.897(7)
W(5)-O(10)	1.911(7)	W(5)-O(7)	1.974(7)	W(5)-O(8)	2.269(7)
W(6)-O(12)	1.717(8)	W(6)-O(11)	1.888(8)	W(6)-O(22)#1	1.888(7)
W(6)-O(10)	1.914(7)	W(6)-O(9)	1.977(7)	W(6)-O(8)	2.316(7)
W(7)-O(24)	1.701(7)	W(7)-O(20)	1.865(7)	W(7)-O(15)	1.898(7)
W(7)-O(21)#1	1.927(7)	W(7)-O(14)	1.998(8)	W(7)-O(13)	2.304(7)
W(8)-O(19)	1.704(7)	W(8)-O(18)	1.906(7)	W(8)-O(15)	1.908(7)
W(8)-O(11)#1	1.910(8)	W(8)-O(16)	1.951(8)	W(8)-O(17)	2.287(7)
As(1)-O(13)	1.679(7)	As(1)-O(17)	1.684(7)	As(1)-O(8)	1.686(7)
As(1)-O(1)	1.703(7)	Cu(5)-N(11)	1.966(9)	Cu(5)-N(9)	1.975(9)
Cu(5)-N(10)	2.042(9)	Cu(5)-Cl(2)#2	2.594(4)	Cu(1)-N(5)	1.965(9)
Cu(1)-N(6)	1.976(10)	Cu(1)-O(25)	2.198(8)	Cu(1)-Cl(1)	2.431(4)
Cu(3)-N(4)#3	1.977(9)	Cu(3)-N(2)	2.044(10)	Cu(3)-Cl(2)	2.266(3)
Cu(3)-O(31)#4	2.627(9)	Cl(2)-Cu(4)#4	2.535(3)	Cu(2)-N(3)	2.010(10)
Cu(2)-N(1)	2.087(11)	Cu(2)-Cl(1)	2.221(3)	Cu(2)-O(23)#5	2.556(8)
Cu(4)-N(7)	1.942(10)	Cu(4)-N(8)	1.981(9)	Cu(4)-O(31)	2.298(8)
Cu(4)-Cl(2)#6	2.535(3)	Cl(2)-Cu(5)#2	2.594(4)	O(29)-W(9)#1	1.912(7)
O(21)-W(7)#1	1.927(7)	O(22)-W(6)#1	1.888(7)	O(13)-W(9)#1	2.340(7)
O(23)-Cu(2)#7	2.556(8)	O(26)-W(5)#1	1.897(7)	O(31)-Cu(3)#6	2.627(8)
As(1)-O(6)-Mo(3)	129.9(3)				
O(19)-W(8)-O(18)	101.3(3)	O(19)-W(8)-O(15)	101.0(3)	O(18)-W(8)-O(15)	157.6(3)
O(19)-W(8)-O(11)#1	98.0(4)	O(18)-W(8)-O(11)#1	89.9(3)	O(15)-W(8)-O(11)#1	88.4(3)
O(19)-W(8)-O(16)	97.2(4)	O(18)-W(8)-O(16)	87.3(3)	O(15)-W(8)-O(16)	88.6(3)
O(11)#1-W(8)-O(16)	164.8(3)	O(19)-W(8)-O(17)	173.6(3)	O(18)-W(8)-O(17)	72.4(3)
O(15)-W(8)-O(17)	85.2(3)	O(11)#1-W(8)-O(17)	83.1(3)	O(16)-W(8)-O(17)	81.8(3)
O(12)-W(6)-O(11)	99.5(4)	O(12)-W(6)-O(22)#1	102.3(3)	O(11)-W(6)-O(22)#1	92.4(3)
O(12)-W(6)-O(10)	100.1(3)	O(11)-W(6)-O(10)	91.1(3)	O(22)#1-W(6)-O(10)	156.4(3)
O(12)-W(6)-O(9)	95.3(3)	O(11)-W(6)-O(9)	165.2(3)	O(22)#1-W(6)-O(9)	85.3(3)
O(10)-W(6)-O(9)	85.4(3)	O(12)-W(6)-O(8)	170.6(3)	O(11)-W(6)-O(8)	84.9(3)
O(22)#1-W(6)-O(8)	85.7(3)	O(10)-W(6)-O(8)	71.4(3)	O(9)-W(6)-O(8)	80.4(3)
O(23)-W(9)-O(22)	102.7(3)	O(23)-W(9)-O(21)	102.1(3)	O(23)-W(9)-O(29)#1	98.6(3)
O(13)-As(1)-O(17)	112.2(3)	O(13)-As(1)-O(1)	106.9(3)	O(8)-As(1)-O(1)	107.0(3)
N(11)-Cu(5)-N(9)	131.9(4)	N(11)-Cu(5)-N(10)	107.5(4)	N(9)-Cu(5)-N(10)	112.2(4)
N(11)-Cu(5)-Cl(2)#2	99.6(3)	N(9)-Cu(5)-Cl(2)#2	102.3(3)	N(5)-Cu(1)-N(6)	145.8(5)
N(5)-Cu(1)-O(25)	94.2(3)	N(6)-Cu(1)-O(25)	92.6(3)	N(5)-Cu(1)-Cl(1)	107.5(3)
O(25)-Cu(1)-Cl(1)	107.6(3)	N(5)-Cu(1)-Cu(2)	108.4(3)	N(4)#3-Cu(3)-N(2)	113.5(4)
N(2)-Cu(3)-Cl(2)	106.4(3)	N(4)#3-Cu(3)-O(31)#4	91.0(4)	N(3)-Cu(2)-N(1)	103.4(4)
N(3)-Cu(2)-Cl(1)	141.6(3)	N(3)-Cu(2)-O(23)#5	95.7(4)	N(1)-Cu(2)-O(23)#5	88.5(4)
Cl(1)-Cu(2)-O(23)#5	101.1(2)	O(31)-Cu(4)-Cl(2)#6	90.9(2)	W(9)-O(23)-Cu(2)#7	149.8(4)

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

Table S2 Selected hydrogen bond lengths ( ) and bond angles (°) of compound **1**

D-H…A	d(D…H)nm	d(H…A)nm	d(D…A)nm	∠(DHA)°
C(2)--H(2)...O(12)#1	0.93	2.51	3.129(16)	124
C(6)--H(6)...O(31)#1	0.93	2.48	3.181(16)	132
C(7)--H(7)...O(19)#2	0.93	2.47	3.229(15)	139
C(8)--H(8)...O(23)#2	0.93	2.58	3.280(16)	132
C(10)--H(10)...O(30)#3	0.93	2.30	3.000(14)	131
C(10)--H(10)...O(4)#4	0.93	2.33	3.102(15)	140
C(17)--H(17)...O(24)#4	0.93	2.40	3.075(15)	129
C(19)--H(19)...O(28)#4	0.93	2.53	3.284(16)	138
C(22)--H(22)...O(24)#4	0.93	2.57	3.085(16)	115

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

Table S3 The BVS calculation result of As, W, and Cu atoms in compound **1**

Code	Bond Valence	Code	Bond Valence
As1	5.260	W8	6.209
W1	6.245	W9	6.181
W2	6.219	Cu1	1.210
W3	6.221	Cu2	0.980
W4	6.017	Cu3	1.006
W5	6.182	Cu4	1.124
W6	6.127	Cu5	1.198
W7	6.190		