A Keggin-type Polyoxometalate-Based Metal−Organic Complex as Highly Efficient Heterogeneous Catalyst for Selective Oxidation of Alkylbenzenes

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Table S1. Bond lengths [Å] and angles [°] for complex 1

Cu(1)-O(3)	2.675(11)	Cu(1)-O(3)#3	2.675(11)
Cu(1)-N(3)#4	1.975(11)	Cu(2)-N(2)#6	1.949(12)
Cu(1)-N(3)	1.975(11)	Cu(3)-N(1)	1.970(11)
Cu(1)-N(3)#1	1.975(11)	Cu(3)-N(1)#1	1.970(11)
Cu(1)-N(3)#5	1.975(11)	Cu(3)-O(3)	2.425(13)
Cu(2)-O(1W)#6	2.001(11)	Cu(3)-O(5)	1.976(10)
Cu(2)-O(1W)	2.001(11)	Cu(3)-O(5)#1	1.976(10)
Cu(2)-N(2)	1.949(12)	N(3)#5-Cu(1)-N(3)	89.3(6)
N(2)-Cu(2)-N(2)#6	180.0(7)	O(1W)-Cu(2)-O(1W)#6	180
N(1)-Cu(3)-N(1)#1	94.6(6)	N(2)-Cu(2)-O(1W)	88.2(5)
N(1)#1-Cu(3)-O(3)	87.9(4)	N(2)#6-Cu(2)-O(1W)#6	88.2(5)
N(1)-Cu(3)-O(3)	87.9(4)	N(2)#6-Cu(2)-O(1W)	91.8(5)
N(1)-Cu(3)-O(5)#1	90.6(4)	N(2)-Cu(2)-O(1W)#6	91.8(5)
N(1)#1-Cu(3)-O(5)	90.6(4)	N(1)#1-Cu(3)-O(5)#1	174.5(4)
N(3)#4-Cu(1)-N(3)#1	89.3(6)	N(1)-Cu(3)-O(5)	174.5(4)
N(3)#1-Cu(1)-N(3)	90.7(6)	O(5)-Cu(3)-O(3)	94.0(4)
N(3)#4-Cu(1)-N(3)	180	O(5)#1-Cu(3)-O(3)	94.0(4)
N(3)#4-Cu(1)-N(3)#5	90.7(6)	O(5)-Cu(3)-O(5)#1	84.1(6)
N(3)#1-Cu(1)-N(3)#5	180.0(6)		

Symmetry code: #1 x,-y+1,z; #3 -x+2,y,-z+2; #4 -x+1,-y+1,-z+1;#5 -x+1,y,-z+1; #6 -x+1/2,-y+1/2,-z+1.

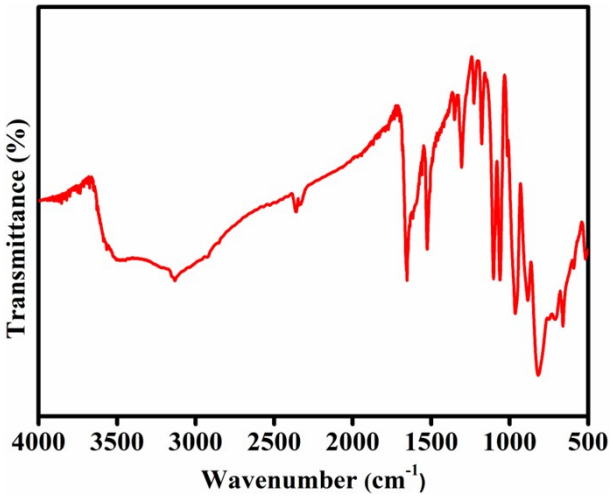

Figure S1. The IR spectrum of complex**1.**

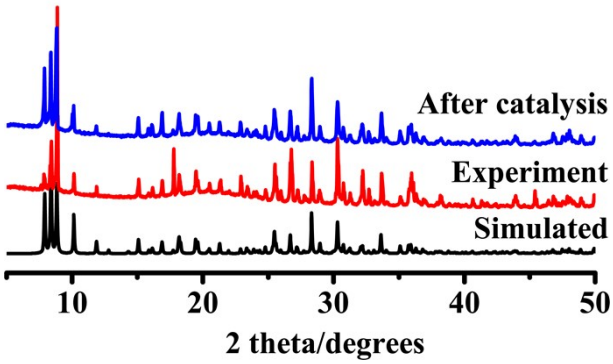

Figure S2. Experiment and simulated X-ray powder diffraction patterns for complex **1**.

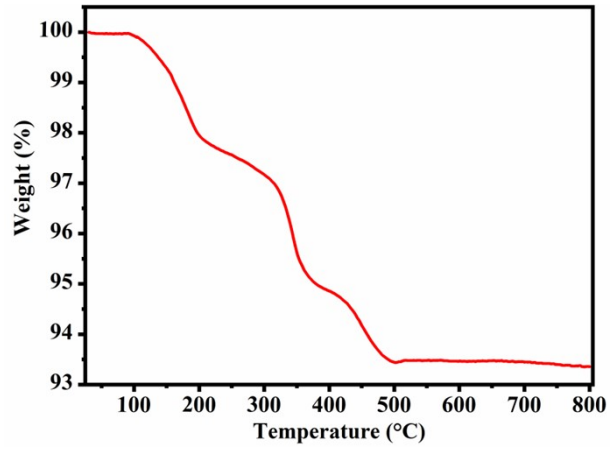

Figure S3. TG curve of complex **1**.

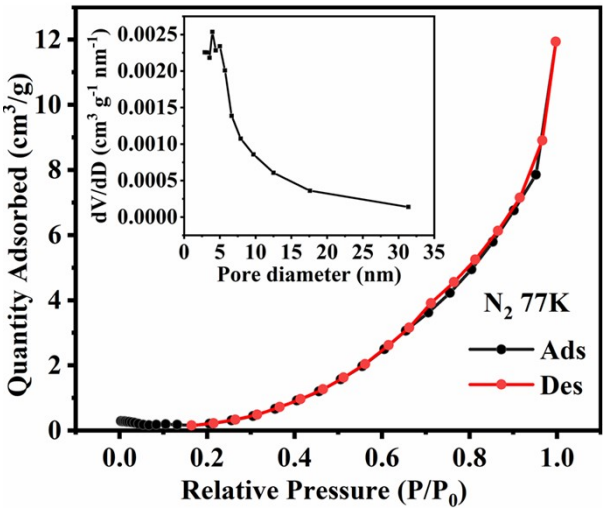

Figure S4. N_2 sorption isotherms of complex **1** at 77 K; P_0 represents 1 atm (inset: the pore size of complex **1**).

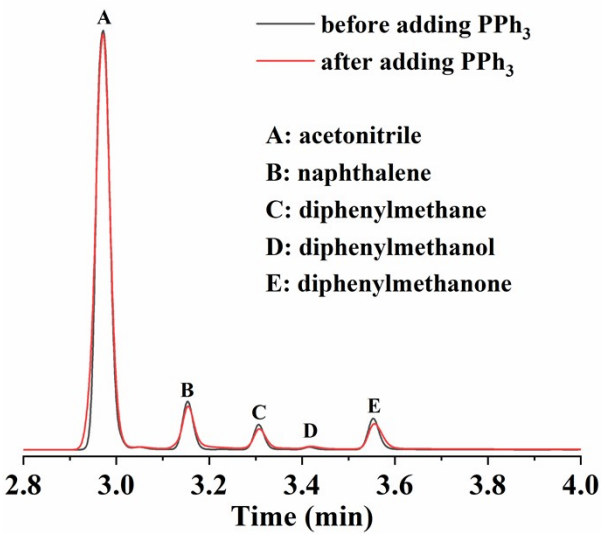

Figure S5. The chromatograms recorded before and after the addition of PPh_3.

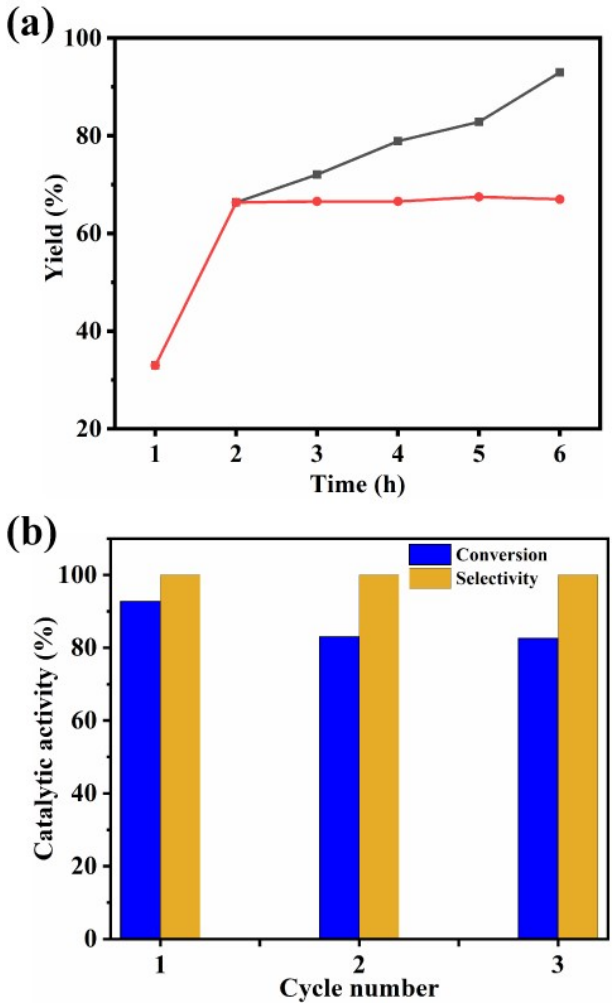

Figure S6. (a) Substrate conversion plotted in the reaction of diphenylmethane with complex **1** (gray) and the leaching test utilizing the hot filtration method (red). **(b)** Recyclability of complex **1** as a catalyst.

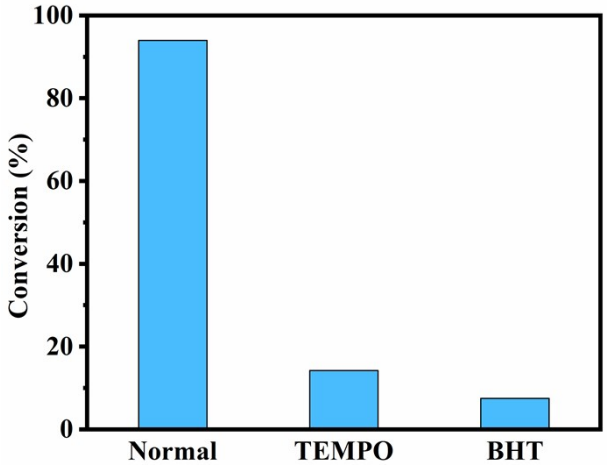

Figure S7. Conversions of diphenylmethane over complex **1** in the presence of different radical scavengers. Reaction conditions: diphenylmethane (0.1 mmol),

TBHP (0.4 mmol), catalyst (1 mol%), CH_3CN (1 mL), TEMPO (0.2 mmol), BHT (0.2 mmol), T = 75 °C, and t = 6 h.