Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Five Keggin-based compounds modified by bis- and mono-[1,3,4]triazole ligands: characterization, selective photocatalytic and electrochemical properties

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Table S1. Selected bond distances (Å) and angles (°) for compounds **1–5**.

Compound **1**

Cu(1)-N(4)	1.985(8)	Cu(1)-N(7)	2.013(8)
Cu(1)-N(2)	1.982(8)	Cu(1)-N(13)	1.989(8)
Cu(1)-O(17)	2.570(4)	Cu(1)-O(29)	2.839(3)
O(17)-Cu(1)-O(29)	169.43(5)	Cu(1)-O(17)-Mo(6)	136.97(5)
N(2)-Cu(1)-N(7)	170.3(4)	N(13)-Cu(1)-N(7)	92.0(3)
N(2)-Cu(1)-N(13)	90.1(3)	N(4)-Cu(1)-N(7)	88.1(4)
N(2)-Cu(1)-N(4)	92.1(3)	N(4)-Cu(1)-N(13)	166.7(4)
N(8)-N(7)-Cu(1)	123.6(7)	N(14)-N(13)-Cu(1)	119.3(6)
C(13)-N(7)-Cu(1)	127.9(8)	C(25)-N(13)-Cu(1)	133.0(7)

Symmetry codes for **1:** #1 -x+2,-y+3,-z+1 #2 -x+2,-y+3,-z+2 #3 -x+3,-y+2,-z+2

Compound **2**

Cu(1)-N(13)	1.996(12)	Cu(1)-N(10)	1.992(14)
Cu(1)-N(7)	2.009(13)	Cu(1)-N(6)	2.008(15)
Cu(1)-O(17)	2.529(4)	Cu(1)-O(29)	2.771(3)
O(17)-Cu(1)-O(29)	169.64(5)	Cu(1)-O(17)-W(6)	128.64(5)
N(13)-Cu(1)-N(7)	168.4(4)	N(10)-Cu(1)-N(7)	91.7(5)
N(13)-Cu(1)-N(10)	90.7(5)	N(10)-Cu(1)-N(6)	171.5(6)
N(13)-Cu(1)-N(6)	91.8(4)	N(6)-Cu(1)-N(7)	87.6(5)
N(14)-N(13)-Cu(1)	118.5(10)	N(8)-N(7)-Cu(1)	120.0(10)
C(25)-N(13)-Cu(1)	131.2(12)	N(11)-N(10)-Cu(1)	116.1(11)

Symmetry codes for **2:** #1 -x+2,-y+3,-z+1 #2 -x+2,-y+3,-z+2 #3 -x+3,-y+2,-z+2

Compound **3**

Cu(1)-N(3)	2.042(10)	Cu(1)-N(4)	2.176(8)

Cu(1)-N(3)#4	2.042(10)	O(15)-Cu(2)	1.850(9)
Cu(1)-N(4) #4	2.176(8)	O(15)-Cu(2)#7	1.850(9)
Cu(1)-N(4)#6	2.176(8)	Cu(2)-N(5)	1.993(7)
N(3)#4-Cu(1)-N(4)	89.3(3)	N(1)#4-Cu(2)-O(15)#9	113.9(5)
N(3)#4-Cu(1)-N(4)#4	89.3(3)	N(1)#4-Cu(2)-O(15)	113.9(6)
N(3)-Cu(1)-N(4)#4	90.2(4)	N(1)#4-Cu(2)-Cu(2)#7	121.5(3)
N(3)#4-Cu(1)-N(4)#4	89.4(4)	O(15)-Cu(2)-O(15)#9	72.91(5)

Symmetry codes for **3:** #1 -x+2,y,-z+3/2 #2 x,y,-z+3/2 #3 -x+2,y,z
#4 -x+1,-y+1,-z+1 #5 -x+1,y,z #6 x,-y+1,-z+1
#7 x,y,-z+1/2 #8 -x+3/2,-y+1/2,-z+1 #9 -x+1,y,-z+1/2

Compound **4**

Cu(1)-N(4)	1.883(4)	Cu(1)-N(5)	1.890(4)
Cu(1)-O(1)	2.694(3)	N(4)-Cu(1)-N(5)	177.58(18)
N(3)-N(4)-Cu(1)	121.4(3)	N(6)-N(5)-Cu(1)	124.0(3)
C(10)-N(4)-Cu(1)	130.7(3)	C(11)-N(5)-Cu(1)	128.1(3)

Symmetry codes for **4:**

Compound **5**

Cu(1)-O(2)	1.933(7)	Cu(1)-N(5)	1.984(10)
Cu(1)-O(2)	2.011(9)	Cu(2)-O(1)	2.601(8)
Cu(2)-O(2)	1.919(8)	Cu(2)-N(1)	1.983(9)
Cu(2)-O(3)	1.887(8)	Cu(2)-N(4)	2.011(9)
Cu(3)-O(3)	1.895(8)	Cu(3)-N(2)	1.985(10)
O(2)-Cu(1)-N(5)	90.2(4)	O(3)-Cu(2)-N(4)	95.0(4)
O(2)-Cu(2)-N(1)	90.9(4)	N(1)-Cu(2)-N(4)	172.2(4)
O(2)-Cu(2)-N(4)	89.8(3)	O(3)-Cu(3)-N(2)	85.0(4)
O(3)-Cu(2)-O(2)	169.1(4)	Cu(2)-O(2)-Cu(1)	107.9(4)
O(3)-Cu(2)-N(1)	85.6(4)	Cu(2)-O(3)-Cu(3)	126.5(4)

Symmetry codes for **5:** #1 -x+1,y,-z+3/2 #2 -x+1/2,-y+1/2,-z+1

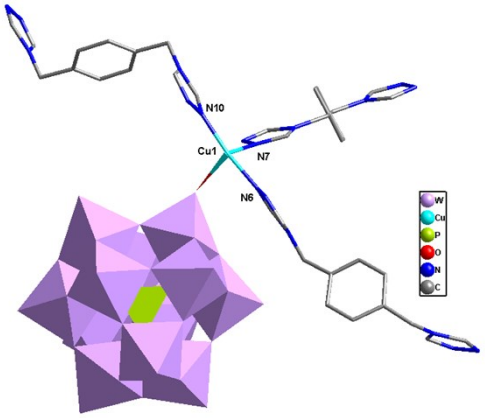


Fig. S1. Polyhedral/stick view of the asymmetric unit of compound **2**. The hydrogen atoms and water molecules are omitted for clarity.

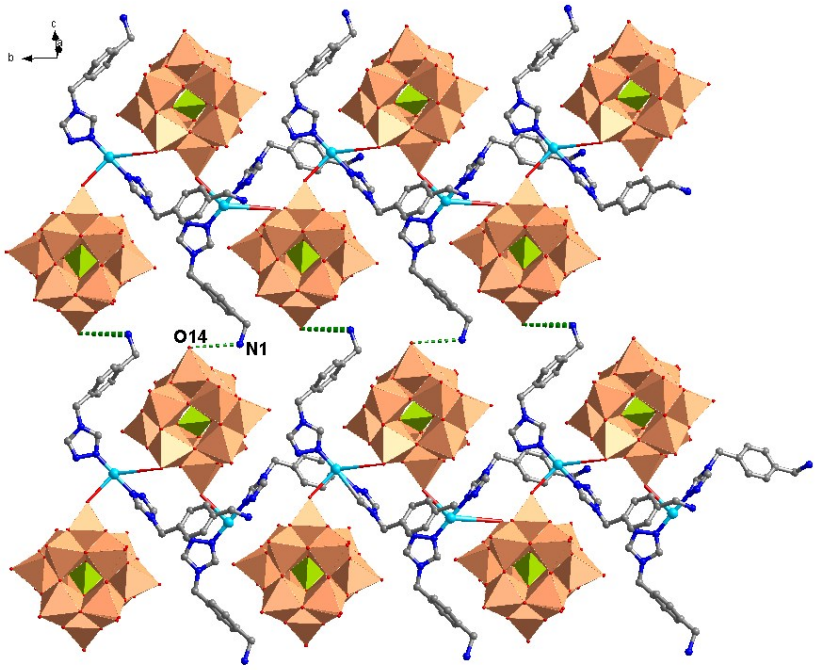


Fig. S2. The 2D supramolecular layer of compound **4**.

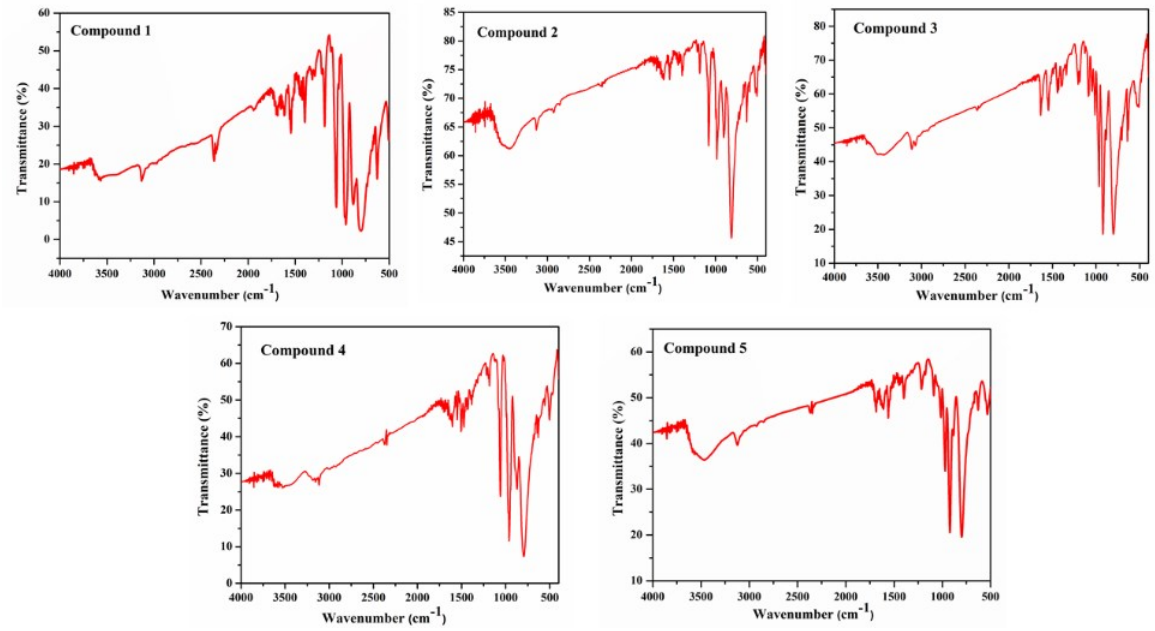
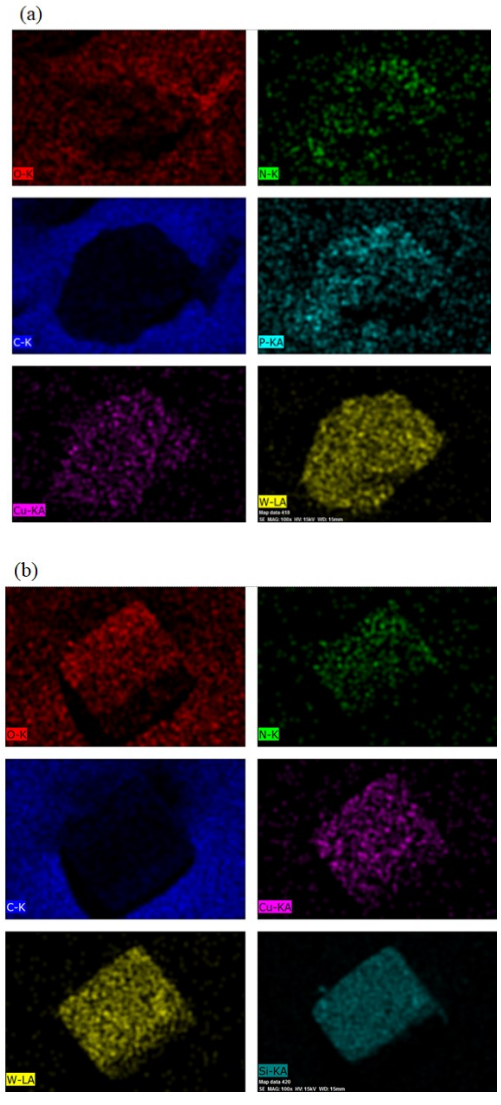


Fig. S3. The IR spectra of compounds **1**−**5**.



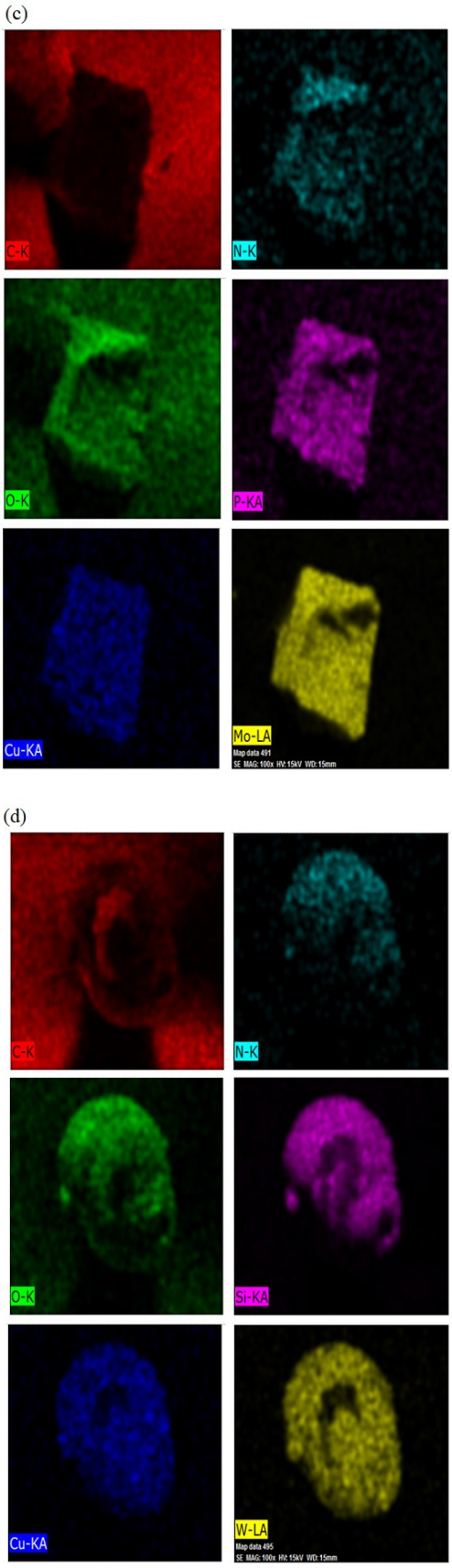


Fig. S4. The elemental mapping images of compound **2**(a), **3**(b), **4**(c) and **5**(d).

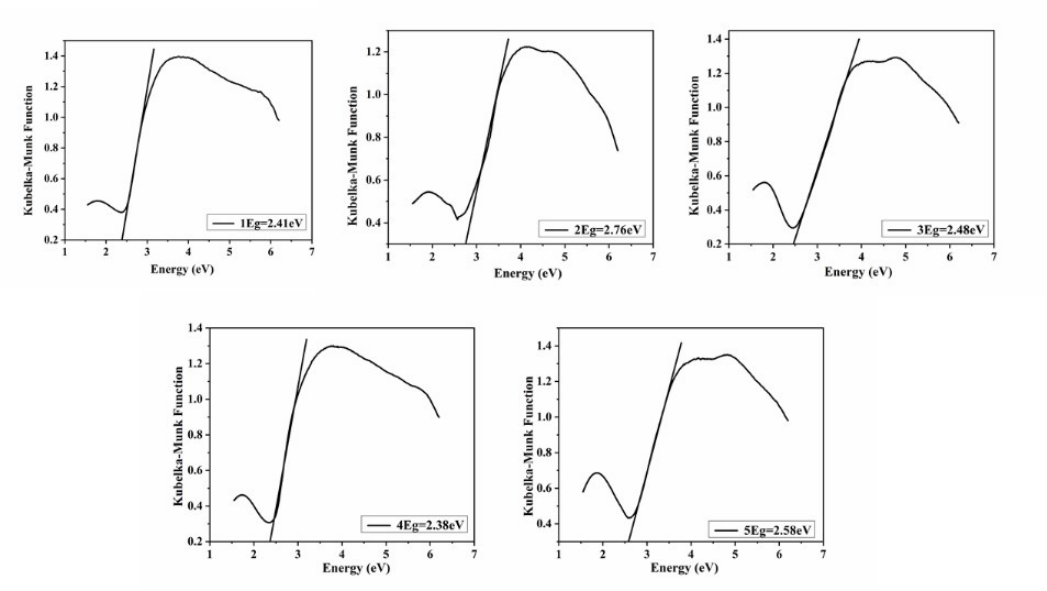


Fig. S5. Solid-state optical diffuse-reflection spectra of compounds **1**−**5** derived from diffuse reflectance data at room temperature.

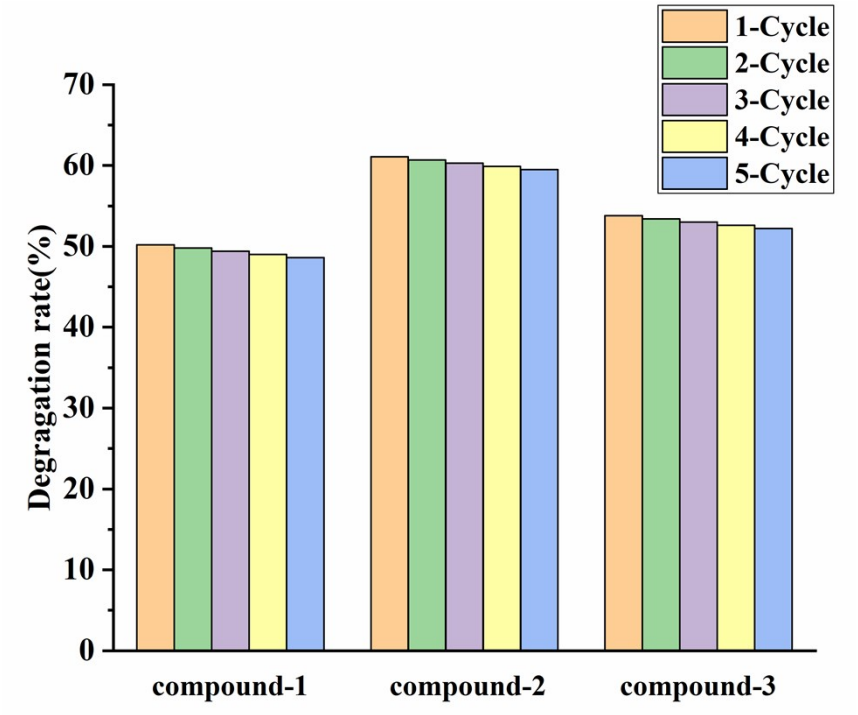


Fig. S6. Degradation rates of compounds **1**–**3** as catalysts in cyclic test.

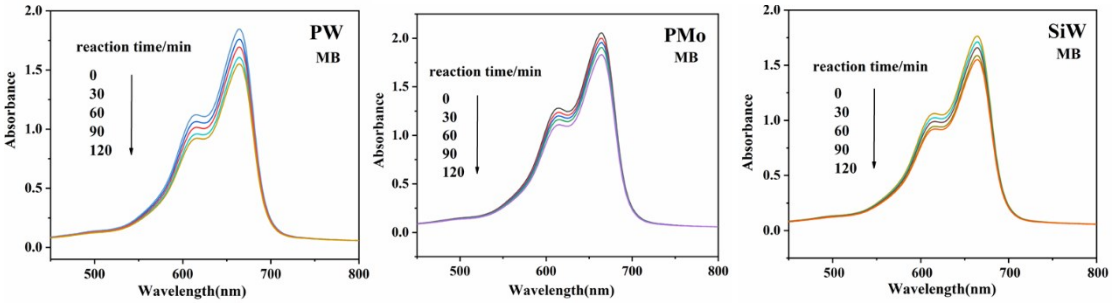


Fig. S7. Absorption spectra of the MB solution during the decomposition reaction under UV irradiation with the pure POMs as the catalysts.

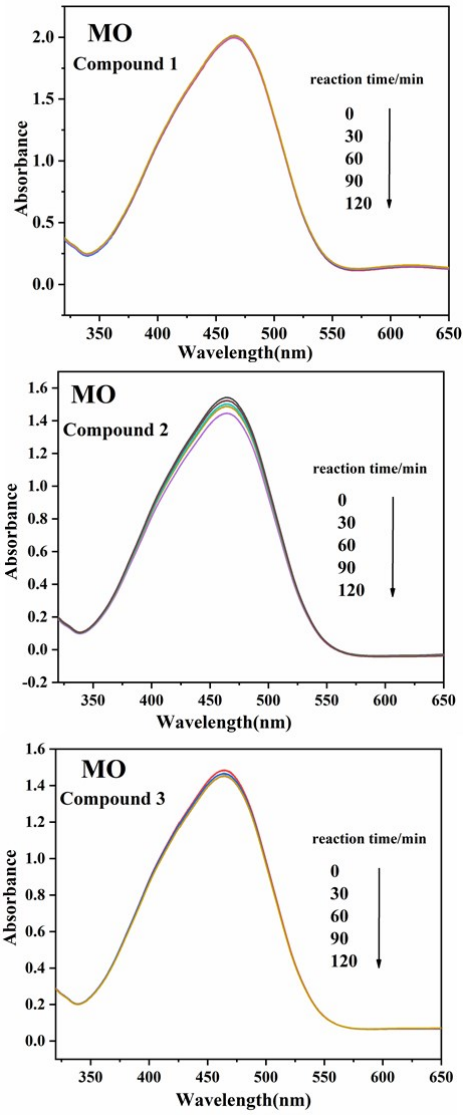


Fig. S8. Absorption spectra of the MO solution during the decomposition reaction under UV irradiation with the compounds **1**–**3** as the catalyst.