Supporting Information for

Designed synthesis of a series of zwitterion-polyoxometalate hybrid materials for selective scavenging and photolysis of dyes

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Figures:

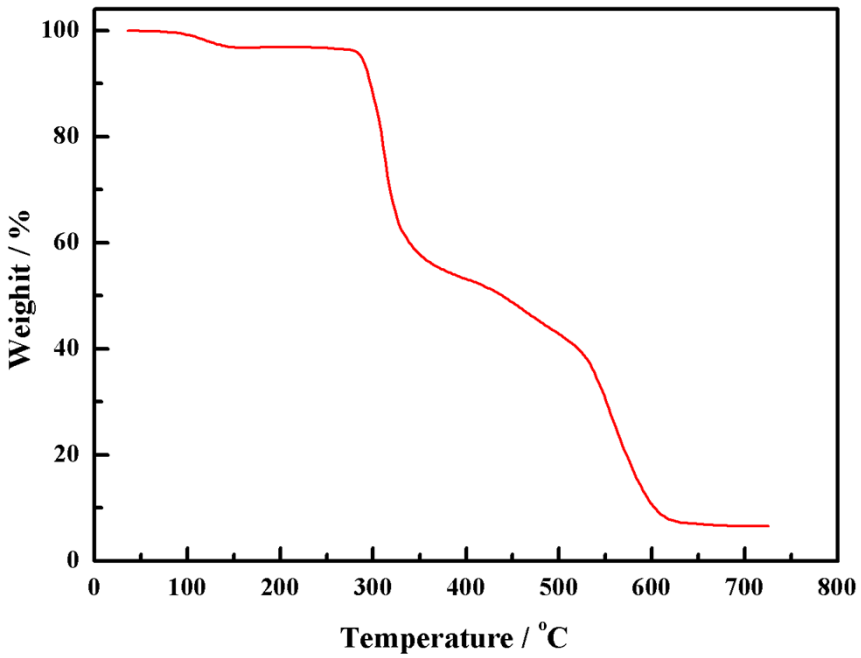

Fig. S1. TGA result of **1**.

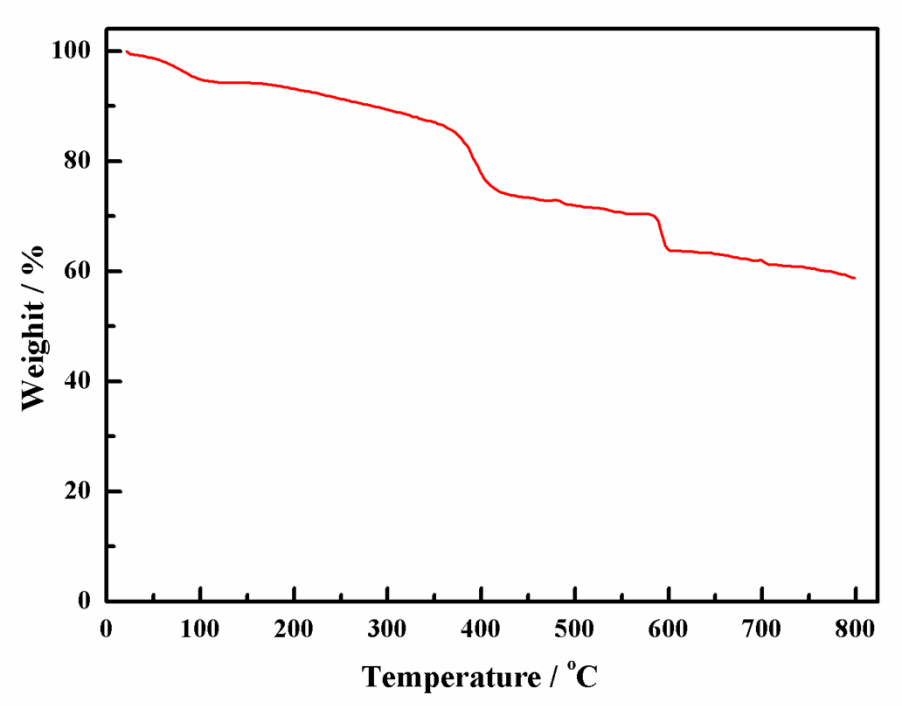

Fig. S2. TGA result of **2**.

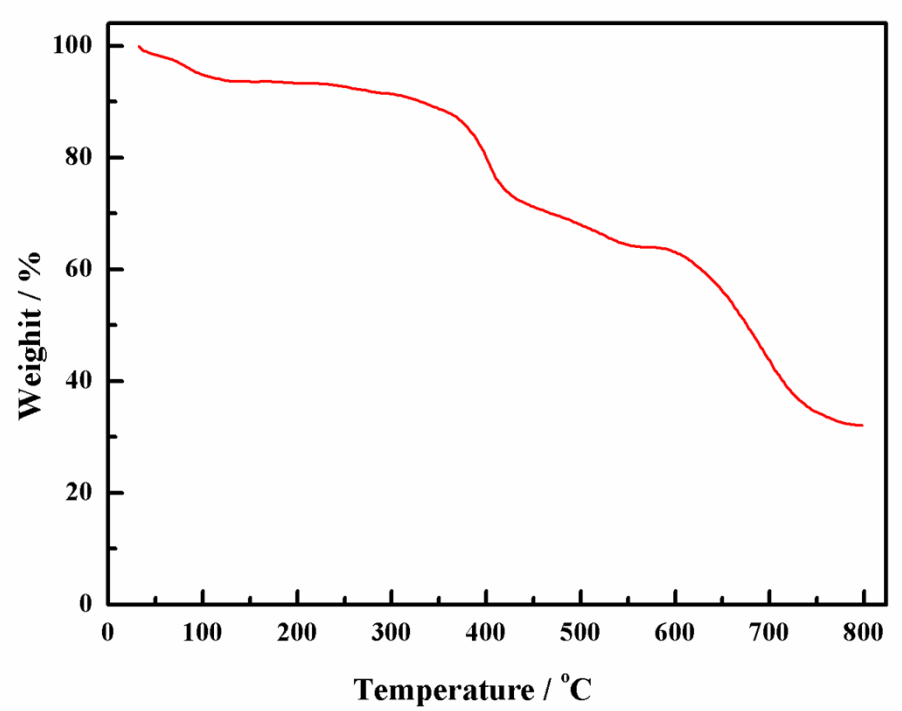

Fig. S3. TGA result of **3**.

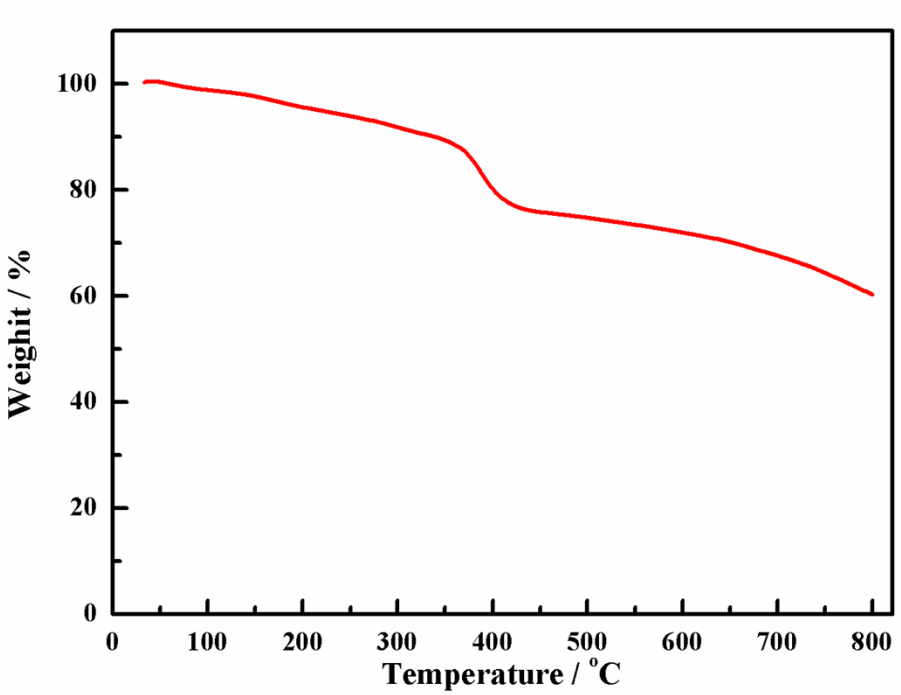

Fig. S4. TGA result of **4**.

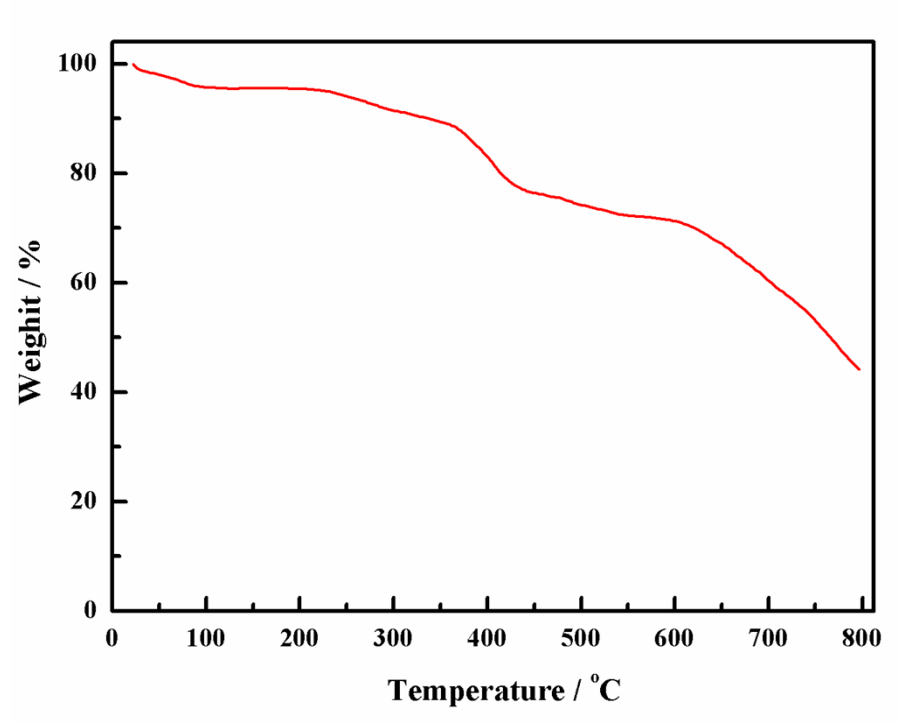

Fig. S5. TGA result of **5**.

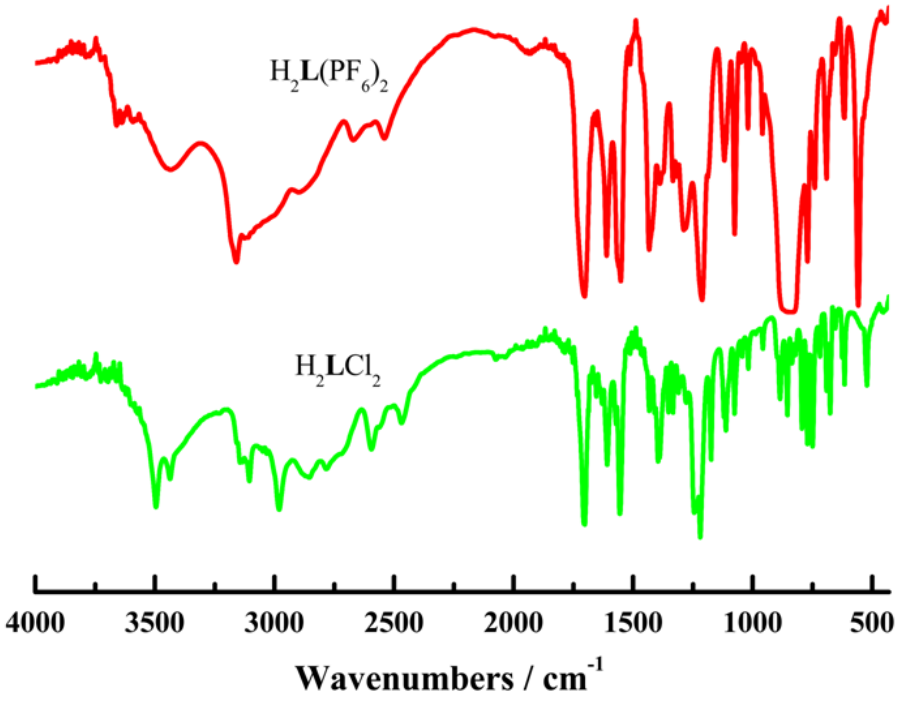

Fig. S6. FT-IR spectra of H_2**L**Cl_2 and H_2**L**PF_6.

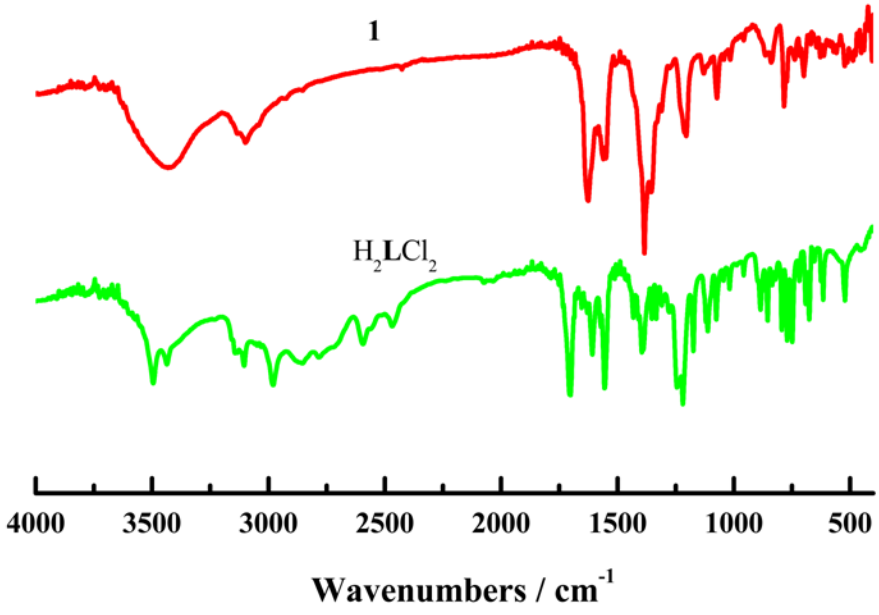

Fig. S7. FT-IR spectra of compound **1** and H_2**L**Cl_2.

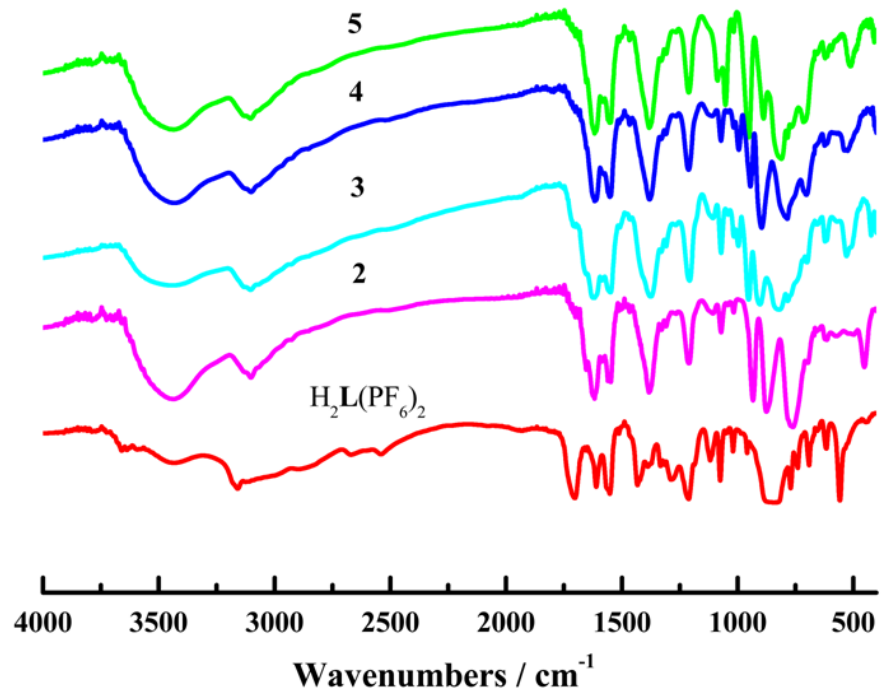

Fig. S8. FT-IR spectra for compounds **2-5** and H_2LPF_6.

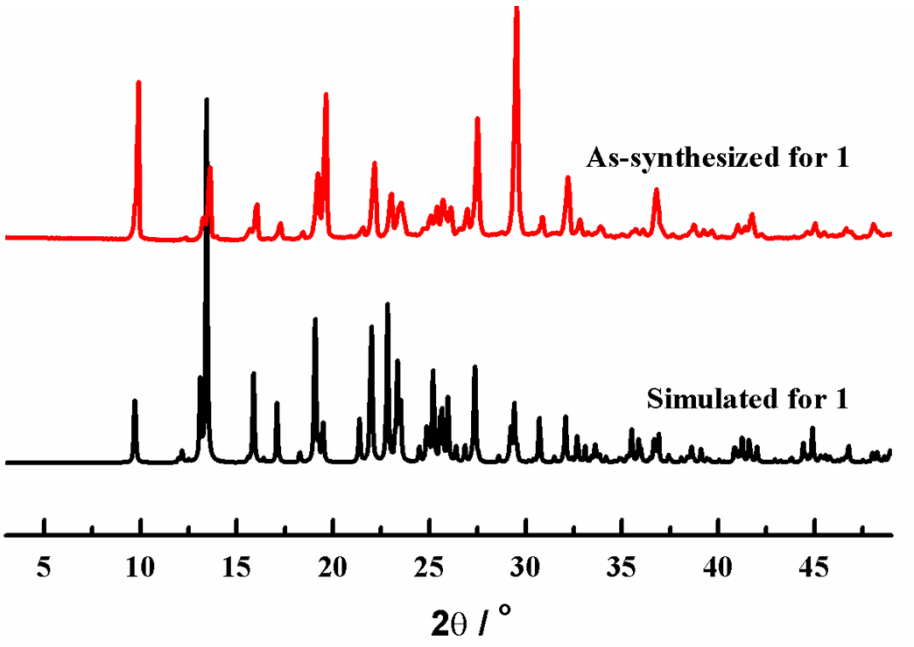

Fig. S9. Powder X-ray diffraction patterns for **1**.

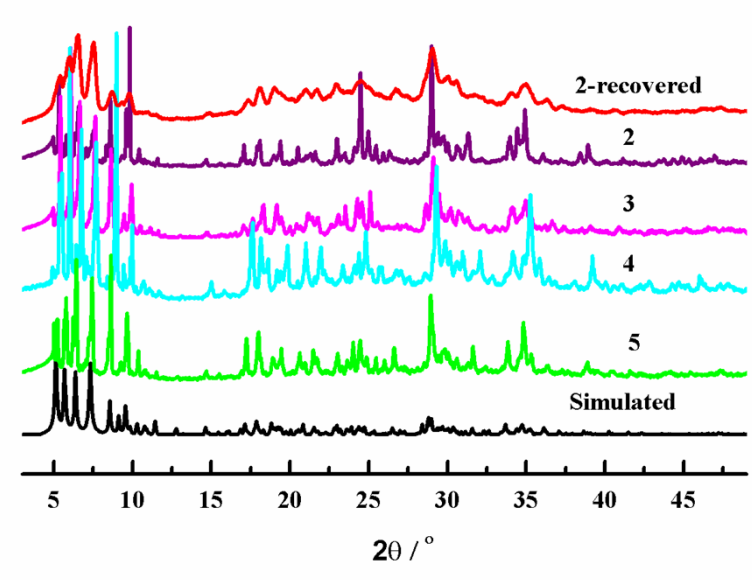

Fig. S10. Powder X-ray diffraction patterns for **2-5**.

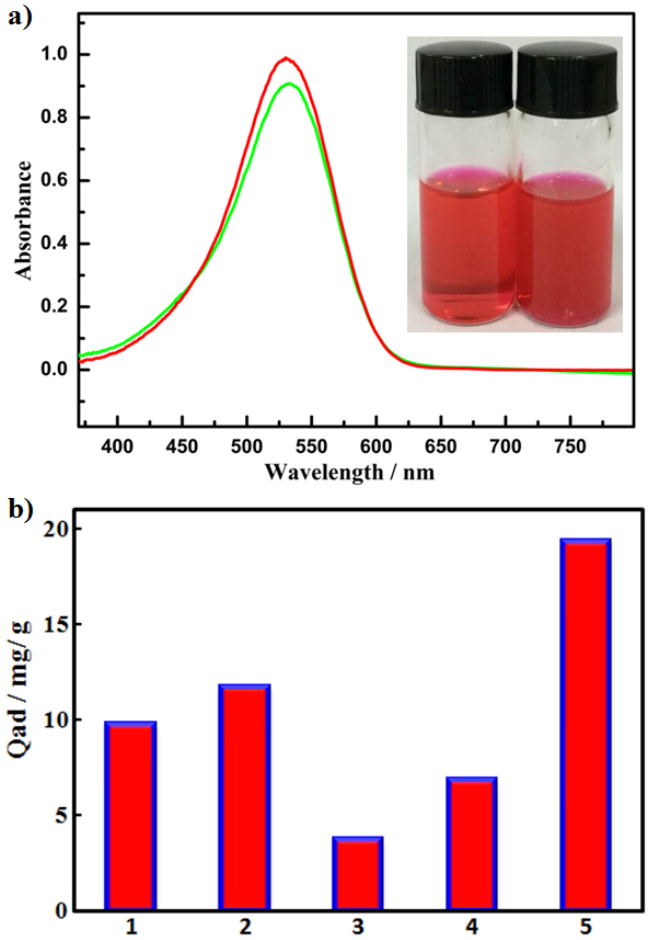

Fig. S11. (a) UV-Vis spectra of NR before (red line) and after (green line) addition of compound **2** (the inserted pictures highlight the scavenging effect); (b) neutral red capture capacities of **1-5**.

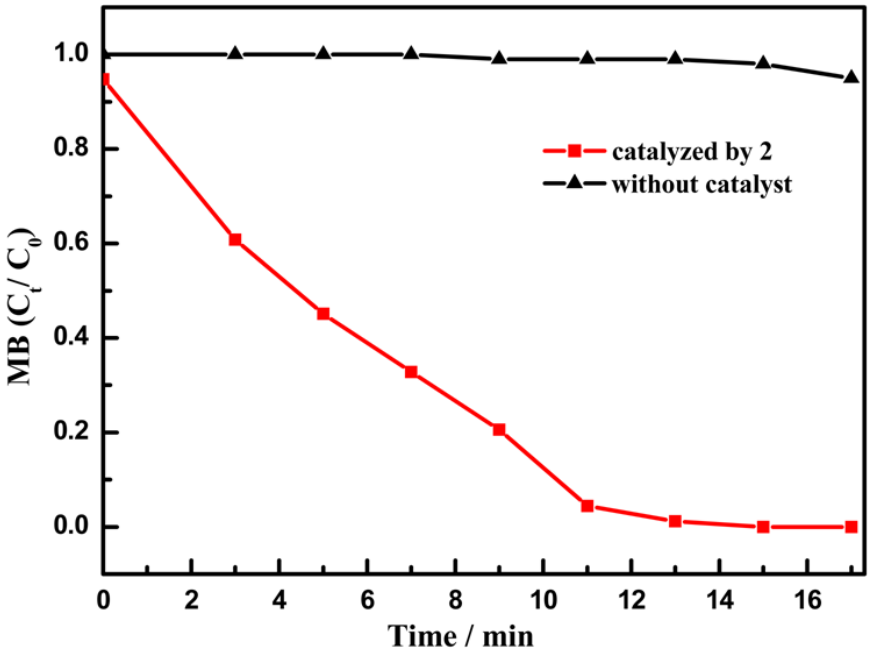

Fig. S12. Photocatalytic property of compound **2** for degradation of MB in water under a 300 W Xe lamp irradiation.

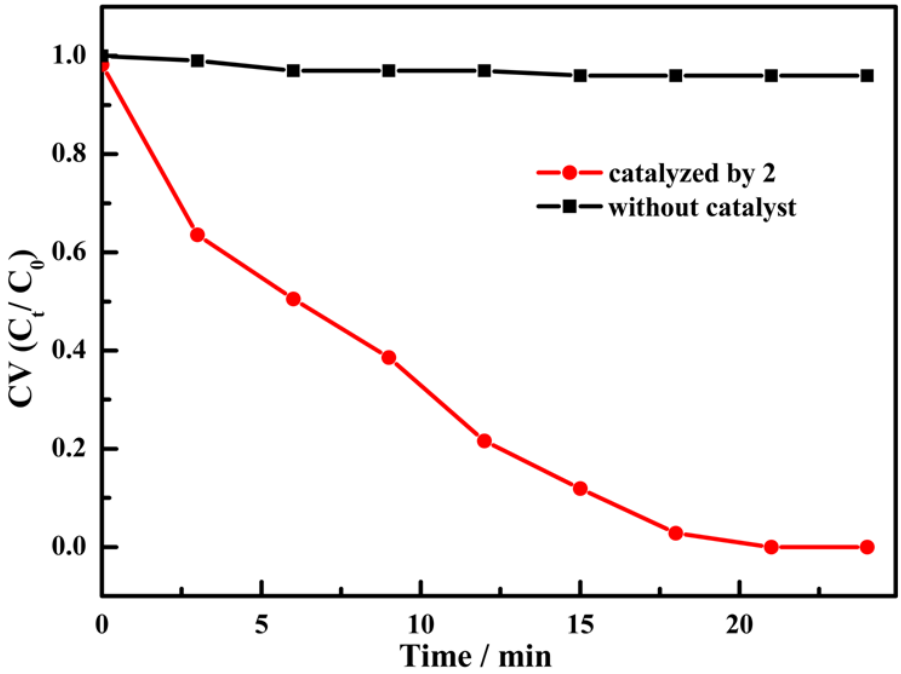

Fig. S13. Photocatalytic property of compound **2** for degradation of CV in water under a 300 W Xe lamp irradiation.

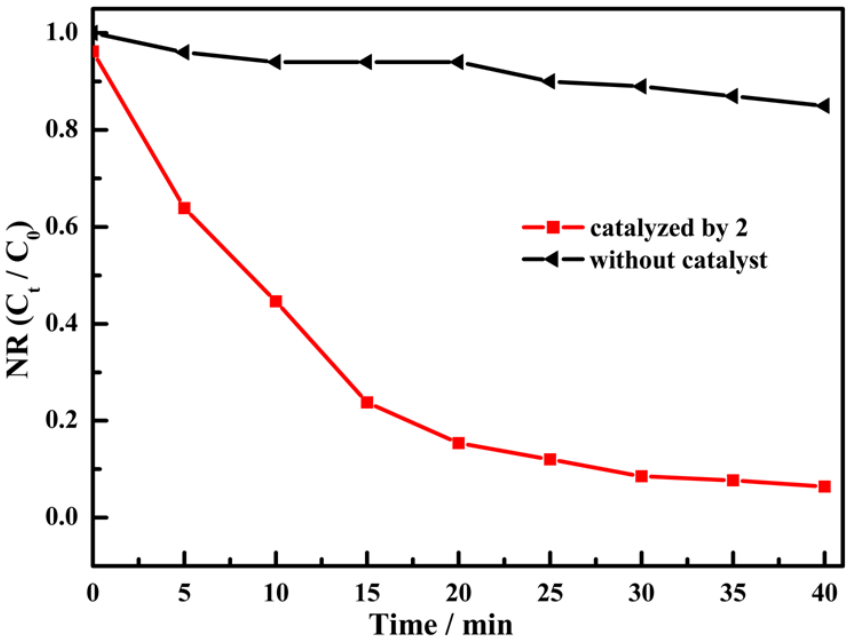

Fig. S14. Photocatalytic property of compound **2** for degradation of NR in water under a 300 W Xe lamp irradiation.

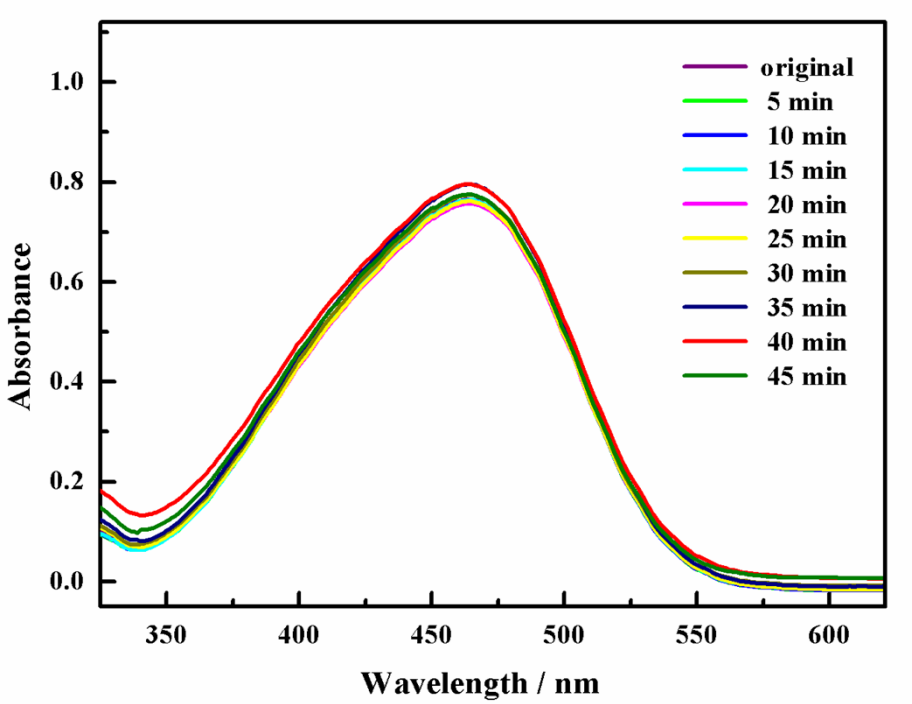

Fig. S15. UV-Vis spectra of MO in water after irradiated with a 300 W Xe lamp in the presence of compound **2**.

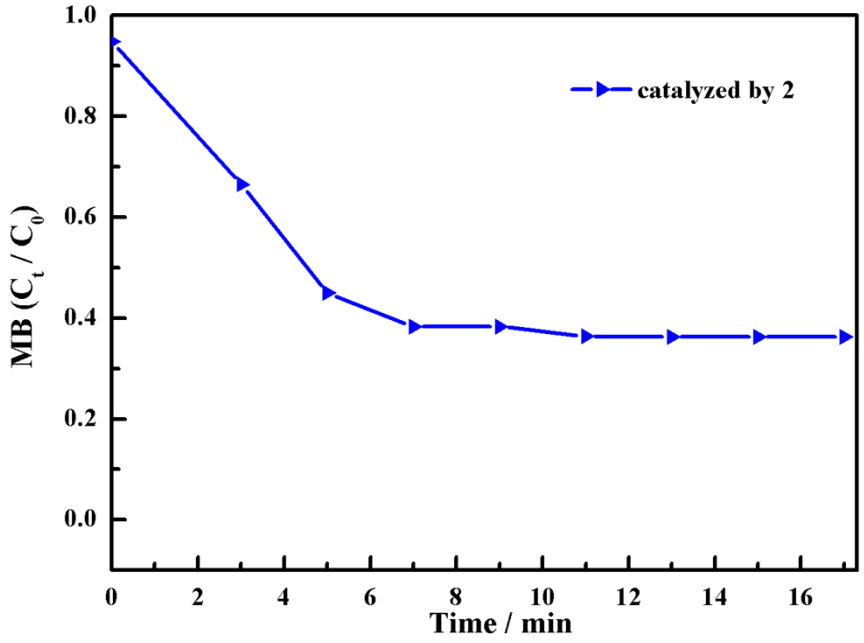

Fig. S16. Photolysis of MB catalyzed by compound **2** under a 300 W Xe lamp irradiation (after 7 min, the solid catalyst was removed by centrifugation).

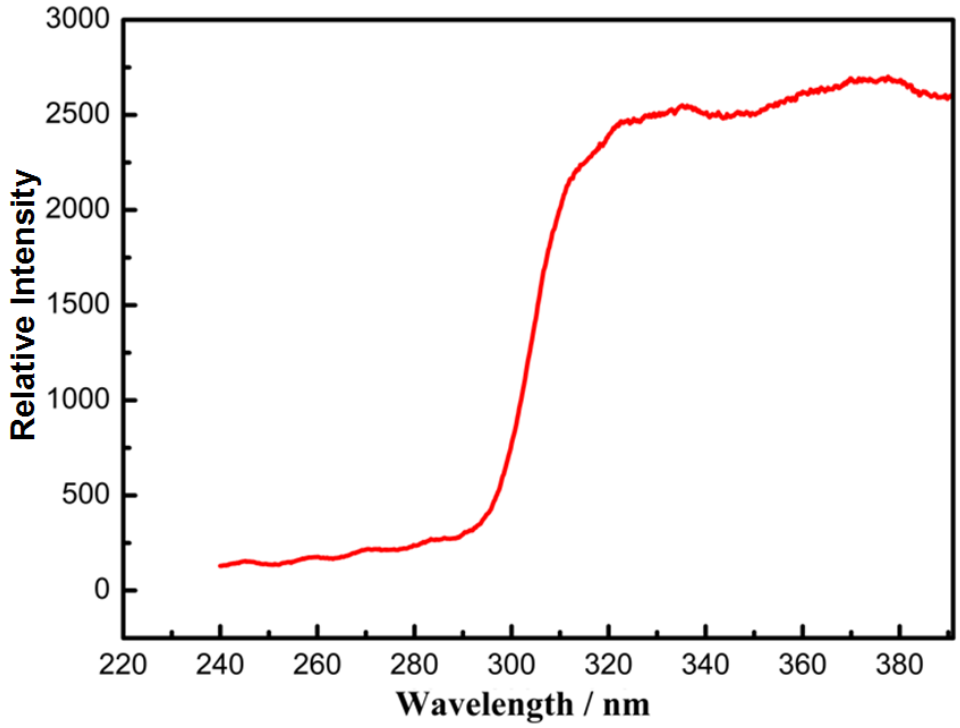

Fig. S17. The excitation spectrum of H_2**L** in the solid state at room temperature (monitored at 444 nm).

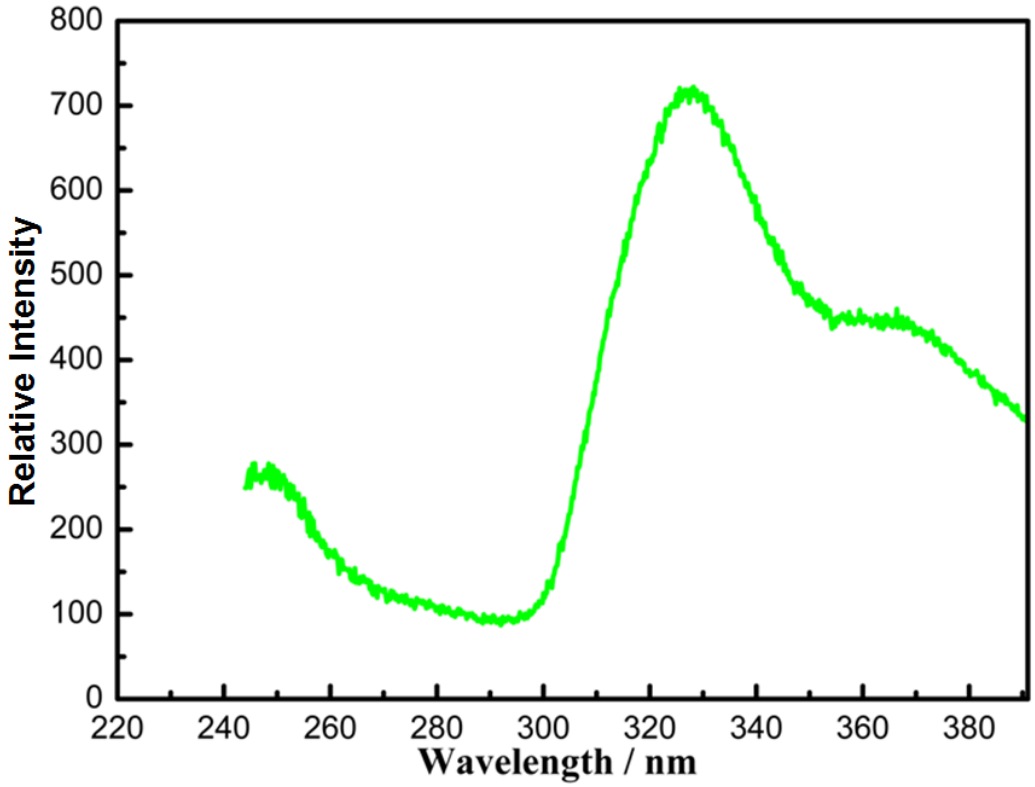

Fig. S18. The excitation spectrum of compound **1** in the solid state at room temperature (monitored at 444 nm).

Tables:

Table S1. Selected bond lengths (Å) and angles (°) for **1**

Bond length	(Å)	Bond angle	(°)	Bond angle	(°)
Zn(1)-O(1)	1.970(5)	O(1)^{i}-Zn(1)-O(1)	91.3(3)	O(1)-Zn(1)-Cl(1)	106.18(17)
Zn(1)-Cl(2)	2.260(3)	O(1)^{i}-Zn(1)-Cl(2)	113.44(17)	Cl(2)-Zn(1)-Cl(1)	121.81(11)
Zn(1)-Cl(1)	2.279(3)				

Symmetry transformations used to generate equivalent atoms: i) x,-y+3/2, z.

Table S2. Selected bond lengths (Å) and angles (°) for **2**

Bond length	(Å)	Bond angle	(°)	Bond angle	(°)
W(1)-O(6)	1.75(2)	O(6)-W(1)-O(17)	100.4(9)	O(4)-W(4)-O(16)	87.2(8)
W(1)-O(17)	1.851(17)	O(6)-W(1)-O(16)	101.3(9)	O(19)-W(4)-O(10)	103.3(9)
W(1)-O(16)	1.911(16)	O(6)-W(1)-O(9)	104.3(10)	O(16)-W(4)-O(10)	86.1(7)
W(1)-O(9)	1.926(19)	O(17)-W(1)-O(9)	87.6(6)	O(19)-W(4)-O(8)	101.0(9)
W(1)-O(13)	1.98(2)	O(16)-W(1)-O(9)	86.9(7)	O(4)-W(4)-O(8)	88.7(9)
W(2)-O(20)	1.58(2)	O(6)-W(1)-O(13)	103.8(10)	O(10)-W(4)-O(8)	87.8(9)
W(2)-O(9)	1.87(2)	O(17)-W(1)-O(13)	86.9(7)	O(4)-W(4)-O(2)	89.5(9)
W(2)-O(14)	1.88(2)	O(16)-W(1)-O(13)	88.2(7)	O(8)-W(4)-O(2)	93.9(7)
W(2)-O(10)	1.88(2)	O(16)-W(1)-O(1)	92.5(7)	O(16)-W(4)-O(22)^{i}	94.3(7)
W(2)-O(18)^{i}	1.93(2)	O(9)-W(1)-O(1)	91.0(8)	O(10)-W(4)-O(22)^{i}	93.5(8)
W(3)-O(15)	1.729(18)	O(17)-W(1)-O(2)	93.2(7)	O(7)-W(5)-O(11)	102.9(9)
W(3)-O(8)	1.84(2)	O(13)-W(1)-O(2)	87.9(8)	O(7)-W(5)-O(12)^{i}	100.6(9)
W(3)-O(18)	1.84(2)	O(20)-W(2)-O(9)	101.7(9)	O(7)-W(5)-O(4)	103.8(9)
W(3)-O(3)^{i}	1.870(16)	O(20)-W(2)-O(14)	99.2(9)	O(11)-W(5)-O(4)	86.9(9)
W(3)-O(11)	1.93(2)	O(20)-W(2)-O(10)	103.2(9)	O(12)^{i}-W(5)-O(4)	86.3(10)
W(4)-O(19)	1.615(19)	O(9)-W(2)-O(10)	85.8(7)	O(7)-W(5)-O(17)^{i}	102.1(8)
W(4)-O(4)	1.84(2)	O(14)-W(2)-O(10)	87.9(8)	O(11)-W(5)-O(17)^{i}	88.5(8)
W(4)-O(16)	1.885(18)	O(20)-W(2)-O(18)^{i}	102.2(9)	O(12)^{i}-W(5)-O(17)^{i}	87.8(8)
W(4)-O(10)	1.90(2)	O(9)-W(2)-O(18)^{i}	87.1(7)	O(12)^{i}-W(5)-O(22)^{i}	92.5(8)
W(4)-O(8)	1.98(2)	O(14)-W(2)-O(18)^{i}	90.1(8)	O(17)^{i}-W(5)-O(22)^{i}	92.5(7)
W(5)-O(7)	1.731(17)	O(9)-W(2)-O(21)	93.4(7)	O(11)-W(5)-O(1)^{i}	92.4(8)
W(5)-O(11)	1.87(2)	O(10)-W(2)-O(21)	92.1(8)	O(4)-W(5)-O(1)^{i}	92.3(9)
W(5)-O(12)^{i}	1.887(19)	O(15)-W(3)-O(8)	100.8(10)	O(5)-W(6)-O(3)	102.2(5)
W(5)-O(4)	1.91(2)	O(15)-W(3)-O(18)	103.6(9)	O(5)-W(6)-O(14)	100.6(6)
W(5)-O(17)^{i}	1.954(18)	O(15)-W(3)-O(3)^{i}	103.0(7)	O(3)-W(6)-O(14)	87.1(7)
W(6)-O(5)	1.72(3)	O(8)-W(3)-O(3)^{i}	86.9(8)	O(3)-W(6)-O(21)^{i}	91.9(7)
W(6)-O(3)	1.918(16)	O(18)-W(3)-O(3)^{i}	87.6(8)	O(14)-W(6)-O(21)^{i}	94.1(8)
W(6)-O(14)	1.97(2)	O(15)-W(3)-O(11)	101.3(8)	O(23)-W(7)-O(13)	104.5(6)
W(7)-O(23)	1.63(3)	O(8)-W(3)-O(11)	89.2(9)	O(23)-W(7)-O(12)	103.1(6)
W(7)-O(13)	1.75(3)	O(18)-W(3)-O(11)	86.2(9)	O(13)-W(7)-O(12)	87.8(8)
W(7)-O(12)	1.890(19)	O(18)-W(3)-O(22)^{i}	90.3(8)	O(24)^{ii}-Zn(1)-O(24)^{iii}	112.1(8)
Zn(1)-O(24)^{ii}	1.975(13)	O(3)^{i}-W(3)-O(22)^{i}	93.3(7)	O(24)^{ii}-Zn(1)-O(27)	106.4(7)
Zn(1)-O(27)	1.996(17)	O(19)-W(4)-O(4)	102.6(10)	O(24)^{iii}-Zn(1)-O(27)	102.8(7)

		O(19)-W(4)-O(16)	101.9(7)	$O(27)^{i}$-Zn(1)-O(27)	126.5(10)

Symmetry transformations used to generate equivalent atoms: i) -x+1, y, -z+1/2; ii) -x+3/2, y+1/2, -z+1/2; iii) x-1/2, y+1/2, z.

Table S3. Selected bond lengths (Å) and angles (°) for **3**

Bond length	(Å)	Bond angle	(°)	Bond angle	(°)
W(1)-O(6)	1.73(3)	O(6)-W(1)-O(13)	100.7(13)	O(19)-W(4)-O(4)	100.9(10)
W(1)-O(13)	1.87(2)	O(6)-W(1)-O(17)	102.9(13)	O(16)-W(4)-O(4)	88.0(8)
W(1)-O(17)	1.868(17)	O(13)-W(1)-O(17)	87.8(7)	O(19)-W(4)-O(8)	100.1(8)
W(1)-O(9)	1.88(2)	O(6)-W(1)-O(9)	102.5(12)	O(4)-W(4)-O(8)	88.2(7)
W(1)-O(16)	1.922(19)	O(17)-W(1)-O(9)	88.6(6)	O(19)-W(4)-O(10)	99.5(10)
W(2)-O(20)	1.652(16)	O(6)-W(1)-O(16)	102.7(11)	O(16)-W(4)-O(10)	86.4(7)
W(2)-O(10)	1.845(19)	O(13)-W(1)-O(16)	87.7(7)	O(8)-W(4)-O(10)	89.5(7)
W(2)-O(9)	1.86(2)	O(9)-W(1)-O(16)	85.6(7)	O(4)-W(4)-O(2)	93.0(7)
W(2)-O(14)	1.93(2)	O(9)-W(1)-O(1)	90.6(9)	O(8)-W(4)-O(2)	95.1(6)
$W(2)-O(18)^{i}$	1.93(2)	O(16)-W(1)-O(1)	90.7(8)	$O(16)-W(4)-O(22)^{i}$	93.5(7)
W(3)-O(15)	1.613(17)	O(13)-W(1)-O(2)	92.1(8)	$O(10)-W(4)-O(22)^{i}$	93.7(8)
$W(3)-O(3)^{i}$	1.825(18)	O(17)-W(1)-O(2)	93.6(10)	O(7)-W(5)-O(4)	100.4(8)
W(3)-O(8)	1.860(19)	O(20)-W(2)-O(10)	100.8(8)	$O(7)-W(5)-O(17)^{i}$	101.5(10)
W(3)-O(18)	1.86(2)	O(20)-W(2)-O(9)	100.6(8)	O(7)-W(5)-O(11)	99.9(8)
W(3)-O(11)	1.899(17)	O(10)-W(2)-O(9)	86.0(8)	O(4)-W(5)-O(11)	87.6(8)
W(4)-O(19)	1.657(19)	O(20)-W(2)-O(14)	102.9(9)	$O(17)^{i}$-W(5)-O(11)	89.4(7)
W(4)-O(16)	1.82(2)	O(10)-W(2)-O(14)	88.8(9)	$O(7)-W(5)-O(12)^{i}$	99.3(9)
W(4)-O(4)	1.89(2)	$O(20)-W(2)-O(18)^{i}$	99.4(9)	$O(4)-W(5)-O(12)^{i}$	91.7(10)
W(4)-O(8)	1.936(17)	$O(9)-W(2)-O(18)^{i}$	87.2(8)	$O(17)^{i}-W(5)-O(12)^{i}$	84.1(8)
W(4)-O(10)	1.96(2)	$O(14)-W(2)-O(18)^{i}$	89.8(7)	$O(4)-W(5)-O(1)^{i}$	98.0(8)
W(5)-O(7)	1.704(16)	O(10)-W(2)-O(21)	97.2(8)	$O(11)-W(5)-O(1)^{i}$	94.2(8)
W(5)-O(4)	1.86(2)	O(9)-W(2)-O(21)	91.0(8)	$O(17)^{i}-W(5)-O(22)^{i}$	93.7(9)
$W(5)-O(17)^{i}$	1.88(2)	$O(15)-W(3)-O(3)^{i}$	101.8(9)	$O(12)^{i}-W(5)-O(22)^{i}$	95.9(9)
W(5)-O(11)	1.887(19)	O(15)-W(3)-O(8)	103.7(8)	O(5)-W(6)-O(14)	99.8(7)
$W(5)-O(12)^{i}$	1.92(2)	$O(3)^{i}-W(3)-O(8)$	85.6(7)	O(5)-W(6)-O(3)	101.1(6)
W(6)-O(5)	1.74(2)	O(15)-W(3)-O(18)	97.0(10)	O(14)-W(6)-O(3)	88.7(8)
W(6)-O(14)	1.86(2)	$O(3)^{i}-W(3)-O(18)$	91.7(8)	$O(14)-W(6)-O(21)^{i}$	95.2(9)
W(6)-O(3)	1.974(17)	O(15)-W(3)-O(11)	98.2(9)	$O(3)-W(6)-O(21)^{i}$	95.6(7)
W(7)-O(23)	1.62(3)	O(8)-W(3)-O(11)	87.6(7)	O(23)-W(7)-O(12)	100.5(7)
W(7)-O(12)	1.85(2)	O(18)-W(3)-O(11)	88.0(8)	O(23)-W(7)-O(13)	101.7(6)
W(7)-O(13)	1.90(2)	$O(8)-W(3)-O(21)^{i}$	94.0(8)	O(12)-W(7)-O(13)	85.0(9)
Zn(1)-O(26)	1.911(18)	$O(11)-W(3)-O(21)^{i}$	93.5(9)	$O(26)^{i}$-Zn(1)-O(26)	123.3(12)
$Zn(1)-O(24)^{ii}$	1.969(12)	$O(3)^{i}-W(3)-O(22)^{i}$	92.5(8)	$O(26)-Zn(1)-O(24)^{ii}$	94.0(7)
		$O(18)-W(3)-O(22)^{i}$	94.8(10)	$O(26)-Zn(1)-O(24)^{iii}$	118.5(7)
		O(19)-W(4)-O(16)	102.7(8)	$O(24)^{ii}$-Zn(1)-$O(24)^{iii}$	109.8(8)

Symmetry transformations used to generate equivalent atoms: i) -x+1, y, -z+1/2; ii) x-1/2, y+1/2, z; iii) -x+3/2, y+1/2, -z+1/2.

Table S4. Selected bond lengths (Å) and angles (°) for **4**

Bond length	(Å)	Bond angle	(°)	Bond angle	(°)
W(1)-O(6)	1.59(2)	O(6)-W(1)-O(9)	103.8(10)	O(19)-W(4)-O(16)	98.1(8)
W(1)-O(9)	1.85(2)	O(6)-W(1)-O(17)	104.5(10)	O(10)-W(4)-O(16)	91.5(8)
W(1)-O(17)	1.86(2)	O(9)-W(1)-O(17)	86.4(7)	O(19)-W(4)-O(8)	103.2(8)
W(1)-O(13)	1.862(18)	O(6)-W(1)-O(13)	96.9(10)	O(10)-W(4)-O(8)	85.7(8)
W(1)-O(16)	1.924(17)	O(17)-W(1)-O(13)	88.9(7)	O(19)-W(4)-O(4)	106.6(10)
W(2)-O(20)	1.61(2)	O(6)-W(1)-O(16)	97.5(10)	O(16)-W(4)-O(4)	87.8(9)
W(2)-O(14)	1.88(2)	O(9)-W(1)-O(16)	88.5(7)	O(8)-W(4)-O(4)	85.0(9)
W(2)-O(9)	1.91(2)	O(13)-W(1)-O(16)	88.3(7)	O(10)-W(4)-O(22)	94.5(9)
W(2)-O(18)^{i}	1.92(2)	O(9)-W(1)-O(1)	94.3(8)	O(16)-W(4)-O(22)	94.3(9)
W(2)-O(10)	1.97(2)	O(16)-W(1)-O(1)	92.3(8)	O(19)-W(4)-O(2)	157.6(7)
W(3)-O(15)	1.628(19)	O(17)-W(1)-O(2)	91.8(8)	O(8)-W(4)-O(2)	94.5(7)
W(3)-O(18)	1.77(2)	O(13)-W(1)-O(2)	94.3(8)	O(4)-W(4)-O(2)	88.1(8)
W(3)-O(3)^{i}	1.794(18)	O(20)-W(2)-O(14)	98.9(9)	O(7)-W(5)-O(4)	104.7(10)
W(3)-O(8)	1.80(2)	O(20)-W(2)-O(9)	103.1(9)	O(7)-W(5)-O(12)^{i}	99.5(9)
W(3)-O(11)	1.95(2)	O(20)-W(2)-O(18)^{i}	104.9(9)	O(4)-W(5)-O(12)^{i}	87.5(11)
W(4)-O(19)	1.594(19)	O(14)-W(2)-O(18)^{i}	87.1(8)	O(7)-W(5)-O(11)	100.1(9)
W(4)-O(10)	1.77(2)	O(9)-W(2)-O(18)^{i}	87.4(7)	O(4)-W(5)-O(11)	86.0(10)
W(4)-O(16)	1.84(2)	O(20)-W(2)-O(10)	101.8(9)	O(7)-W(5)-O(17)^{i}	102.7(9)
W(4)-O(8)	1.915(19)	O(14)-W(2)-O(10)	86.5(7)	O(12)^{i}-W(5)-O(17)^{i}	89.4(8)
W(4)-O(4)	1.92(3)	O(9)-W(2)-O(10)	89.0(7)	O(11)-W(5)-O(17)^{i}	87.9(8)
W(5)-O(7)	1.656(17)	O(9)-W(2)-O(21)	94.5(8)	O(12)^{i}-W(5)-O(22)	93.6(9)
W(5)-O(4)	1.71(3)	O(10)-W(2)-O(21)	92.1(8)	O(17)^{i}-W(5)-O(22)	94.5(9)
W(5)-O(12)^{i}	1.82(2)	O(14)-W(2)-O(2)	95.8(8)	O(5)-W(6)-O(14)	101.0(6)
W(5)-O(11)	1.83(2)	O(18)^{i}-W(2)-O(2)	89.5(8)	O(5)-W(6)-O(3)	102.2(5)
W(5)-O(17)^{i}	1.85(2)	O(15)-W(3)-O(18)	102.7(9)	O(14)-W(6)-O(3)	88.1(7)
W(6)-O(5)	1.59(3)	O(15)-W(3)-O(3)^{i}	101.1(8)	O(14)-W(6)-O(21)^{i}	94.5(8)
W(6)-O(14)	1.86(2)	O(18)-W(3)-O(3)^{i}	89.2(8)	O(3)-W(6)-O(21)^{i}	92.2(7)
W(6)-O(3)	1.933(19)	O(15)-W(3)-O(8)	102.2(9)	O(13)-W(7)-O(12)	88.7(8)
W(7)-O(23)	1.61(3)	O(3)^{i}-W(3)-O(8)	86.5(8)	O(13)^{i}-W(7)-O(1)	95.3(7)
W(7)-O(13)	1.87(2)	O(15)-W(3)-O(11)	101.0(9)	O(12)^{i}-W(7)-O(1)	89.8(8)
W(7)-O(12)	1.92(2)	O(18)-W(3)-O(11)	87.1(9)	O(23)-W(7)-O(13)	101.8(6)
Zn(1)-O(27)	1.93(2)	O(8)-W(3)-O(11)	87.7(8)	O(23)-W(7)-O(12)	102.2(6)
Zn(1)-O(24)^{ii}	1.992(13)	O(8)-W(3)-O(21)^{i}	94.1(8)	O(27)^{i}-Zn(1)-O(27)	127.1(11)
		O(11)-W(3)-O(21)^{i}	94.4(8)	O(27)-Zn(1)-O(24)^{ii}	105.1(7)
		O(18)-W(3)-O(22)	92.7(9)	O(27)-Zn(1)-O(24)^{iii}	104.1(8)
		O(3)^{i}-W(3)-O(22)	94.0(8)	O(24)^{ii}-Zn(1)-O(24)^{iii}	111.2(8)
		O(19)-W(4)-O(10)	100.6(9)		

Symmetry transformations used to generate equivalent atoms: i) -x+1, y, -z+1/2; ii) x-1/2, y+1/2, z; iii) -x+3/2, y+1/2, -z+1/2.

Table S5. Selected bond lengths (Å) and angles (°) for **5**

Bond length	(Å)	Bond angle	(°)	Bond angle	(°)
W(1)-O(6)	1.60(2)	O(6)-W(1)-O(19)	93.6(14)	O(16)-W(4)-O(8)	99.0(12)
W(1)-O(19)	1.68(2)	O(6)-W(1)-O(4)	101.8(14)	O(10)-W(4)-O(8)	88.5(14)
W(1)-O(4)	1.82(3)	O(6)-W(1)-O(18)	96.6(13)	O(16)-W(4)-O(12)	101.2(13)
W(1)-O(18)	1.83(2)	O(19)-W(1)-O(18)	94.0(11)	O(17)-W(4)-O(12)	88.2(14)
W(1)-O(17)	1.89(3)	O(4)-W(1)-O(18)	84.2(11)	O(8)-W(4)-O(12)	85.0(13)
W(1)-O(2)	2.09(4)	O(6)-W(1)-O(17)	103.8(13)	O(10)-W(4)-O(1)	94.0(13)
W(2)-O(20)	1.60(2)	O(19)-W(1)-O(17)	86.7(11)	O(17)-W(4)-O(1)	102.4(9)
W(2)-O(9)	1.81(3)	O(4)-W(1)-O(17)	89.8(11)	O(8)-W(4)-O(21)	103.3(13)
W(2)-O(14)	1.89(2)	O(4)-W(1)-O(2)	97.2(12)	O(12)-W(4)-O(21)	99.3(14)
W(2)-O(4)	1.91(3)	O(17)-W(1)-O(2)	95.7(11)	O(7)-W(5)-O(12)	103.0(12)
W(2)-O(10)	1.98(3)	O(19)-W(1)-O(21)	106.4(13)	O(7)-W(5)-O(11)	96.6(13)
W(3)-O(15)	1.57(2)	O(18)-W(1)-O(21)	105.2(12)	O(12)-W(5)-O(11)	86.4(14)
W(3)-O(3)^{i}	1.78(3)	O(20)-W(2)-O(9)	106.3(12)	O(7)-W(5)-O(13)^{i}	101.9(15)
W(3)-O(9)^{i}	1.81(3)	O(20)-W(2)-O(14)	98.3(12)	O(12)-W(5)-O(13)^{i}	90.7(15)
W(3)-O(8)	1.92(3)	O(9)-W(2)-O(14)	83.7(11)	O(7)-W(5)-O(18)^{i}	97.2(11)
W(3)-O(11)	1.97(3)	O(20)-W(2)-O(4)	103.8(12)	O(11)-W(5)-O(18)^{i}	89.7(10)
W(3)-O(1)	2.06(3)	O(9)-W(2)-O(4)	85.2(12)	O(13)^{i}-W(5)-O(18)^{i}	86.6(11)
W(4)-O(16)	1.616(19)	O(20)-W(2)-O(10)	102.9(11)	O(12)-W(5)-O(2)^{i}	102.3(12)
W(4)-O(10)	1.73(3)	O(14)-W(2)-O(10)	89.2(12)	O(11)-W(5)-O(2)^{i}	102.6(12)
W(4)-O(17)	1.78(3)	O(4)-W(2)-O(10)	90.8(12)	O(13)^{i}-W(5)-O(1)	103.7(12)
W(4)-O(8)	1.85(3)	O(9)-W(2)-O(21)	96.6(13)	O(18)^{i}-W(5)-O(1)	104.0(10)
W(4)-O(12)	1.88(4)	O(14)-W(2)-O(21)	102.3(13)	O(5)-W(6)-O(14)	99.2(8)
W(5)-O(7)	1.58(3)	O(4)-W(2)-O(22)^{i}	100.8(10)	O(5)-W(6)-O(3)	101.4(7)
W(5)-O(12)	1.82(3)	O(10)-W(2)-O(22)^{i}	97.6(10)	O(14)-W(6)-O(3)	85.6(9)
W(5)-O(11)	1.83(3)	O(15)-W(3)-O(3)^{i}	102.2(13)	O(14)-W(6)-O(22)	99.5(11)
W(5)-O(13)^{i}	1.95(4)	O(15)-W(3)-O(9)^{i}	104.7(12)	O(3)-W(6)-O(22)	100.9(10)
W(5)-O(18)^{i}	2.01(2)	O(3)^{i}-W(3)-O(9)^{i}	87.0(11)	O(23)-W(7)-O(13)	99.9(12)
W(6)-O(14)	1.88(2)	O(15)-W(3)-O(8)	102.5(12)	O(23)-W(7)-O(19)	100.2(6)
W(6)-O(3)	1.96(3)	O(3)^{i}-W(3)-O(8)	88.6(10)	O(13)-W(7)-O(19)	87.7(12)
W(6)-O(22)	2.06(3)	O(15)-W(3)-O(11)	98.1(13)	O(13)^{i}-W(7)-O(2)	99.8(14)
W(7)-O(23)	1.57(4)	O(9)^{i}-W(3)-O(11)	88.8(12)	O(19)^{i}-W(7)-O(2)	103.7(12)
W(7)-O(13)	1.78(4)	O(8)-W(3)-O(11)	86.1(11)	O(2)-Co(1)-O(21)^{i}	114(2)
W(7)-O(19)	2.18(2)	O(3)^{i}-W(3)-O(1)	94.0(13)	O(2)-Co(1)-O(1)	112.9(14)
Co(1)-O(2)	1.914(10)	O(9)^{i}-W(3)-O(1)	96.6(12)	O(21)^{i}-Co(1)-O(1)	111.6(17)
Co(1)-O(21)	1.921(10)	O(8)-W(3)-O(22)	97.7(11)	O(21)-Co(1)-O(22)	103.3(18)
Co(1)-O(1)	1.923(10)	O(11)-W(3)-O(22)	105.1(11)	O(1)^{i}-Co(1)-O(22)	100.8(15)
Co(1)-O(22)	1.924(10)	O(16)-W(4)-O(10)	102.6(13)	O(24)^{ii}-Zn(1)-O(24)^{iii}	112.7(12)
Zn(1)-O(24)^{ii}	1.945(19)	O(16)-W(4)-O(17)	102.9(11)	O(24)^{ii}-Zn(1)-O(27)	104.1(10)
Zn(1)-O(27)	1.96(3)	O(10)-W(4)-O(17)	89.3(12)	O(27)^{iv}-Zn(1)-O(27)	127.6(17)

Symmetry transformations used to generate equivalent atoms: i) -x+1, y, -z+1/2; ii) -x+3/2, y-1/2, -z+3/2; iii) x+1/2, y-1/2, z； iv) -x+2, y, -z+3/2.