Supporting Information

Two Ln-based metal-organic frameworks based on5-(1H-1,2,4-triazol-1-yl)-1,3-benzenedicarboxylic acid ligand: Syntheses, structures, and photocatalytic properties
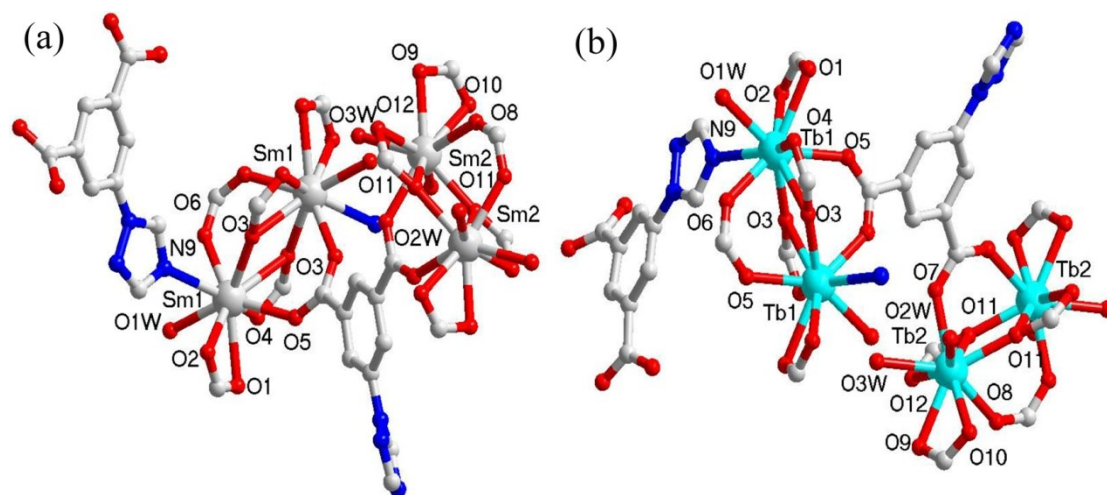

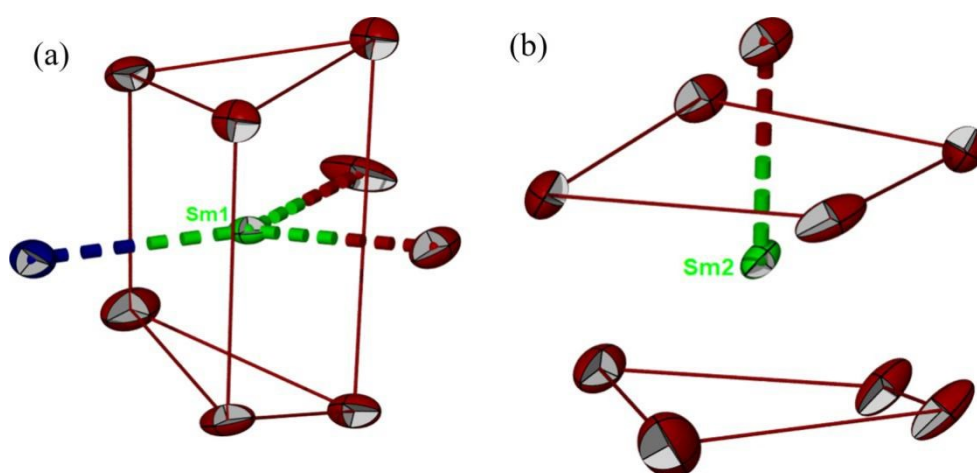Fig. S1 view of the coordination modes of H_2L ligands in **MOF-Sm** and **MOF-Tb**.

Fig. S2 view of the coordination geometries of Sm center in **MOF-Sm**.
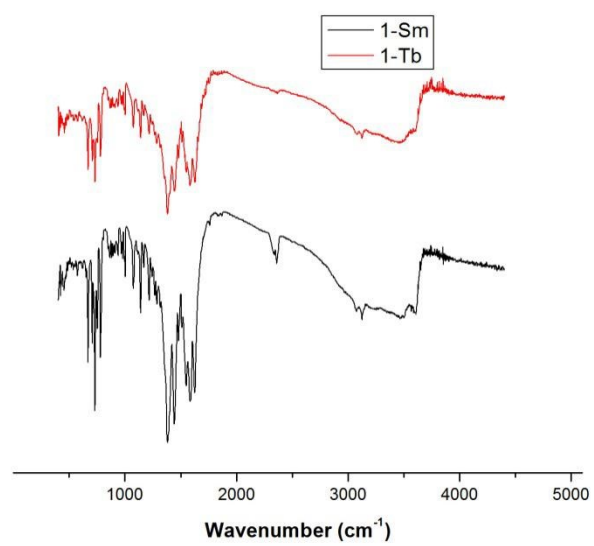
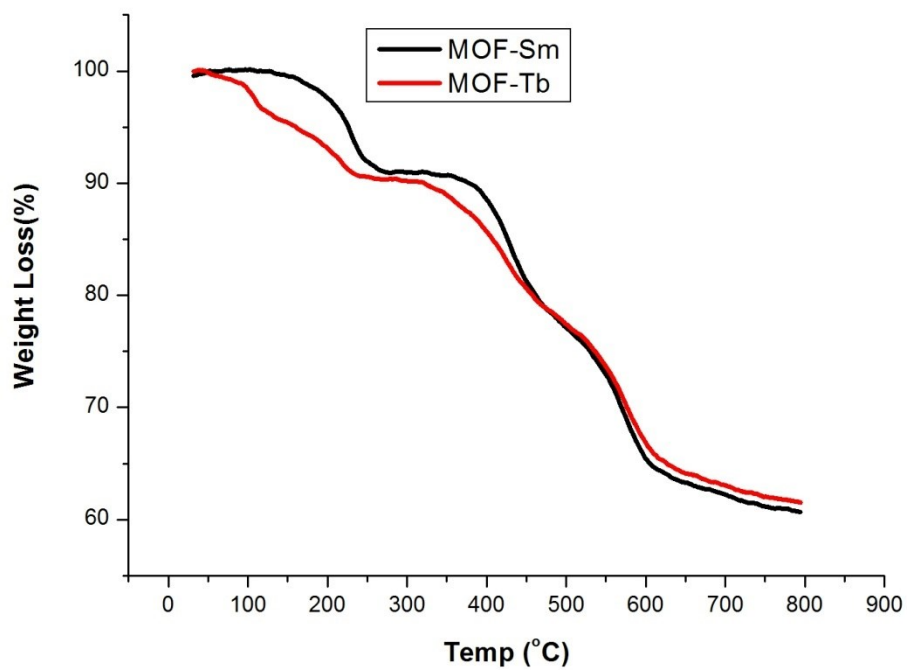Fig. S3 view of the IR of **MOF-Sm** (black) **and MOF-Tb** (red).
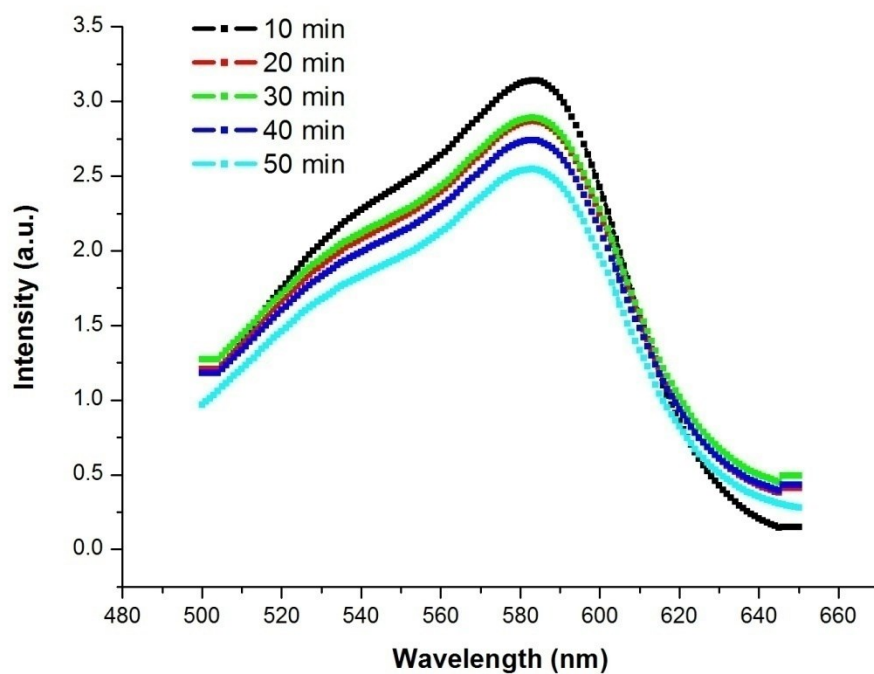
Fig. S4 view of the TGA.

Fig. S5 Absorption spectra of the MV solutions during the decomposition reaction under UV irradiation without any catalysts.
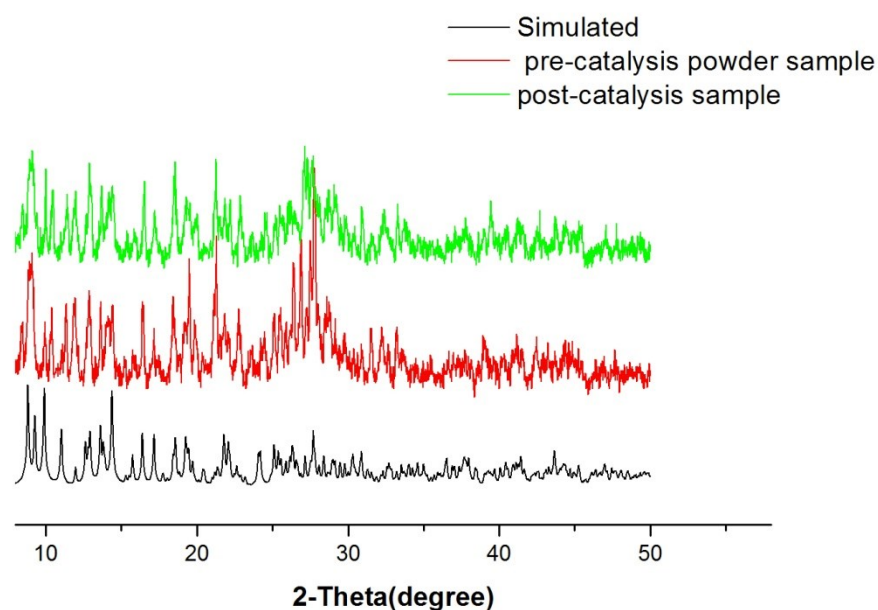
Fig. S6 X-Ray power diffraction diagram of the simulated spectra fromsingle crystal data of **MOF-Sm** (black), **MOF-Sm** (red), and after a photocatalysis process (green).

Table S1. Crystallographic data and structural refinement parameters for MOFs[a]

Compounds	MOF-Sm	MOF-Tb
Empirical formula	$C_{30}H_{27}N_9O_{18}Sm_2$	$C_{30}H_{27}N_9O_{18}Tb_2$
Formula weight	1102.30	1119.44
Crystal system	Triclinic	Triclinic
Space group	P -1	P -1
a /Å	9.9847(8)	9.9419(6)
b /Å	13.2497(10)	13.1775(8)
c /Å	14.3535(11)	14.3215(9)

$\alpha/°$	81.6299(12)	81.7900(9)
$\beta/°$	73.8538(10)	74.0669(9)
$\gamma/°$	83.2186(11)	83.0217(10)
$V/Å^3$	1798.5(2)	1778.99(19)
Z	2	2
ρ_{calc} (g·cm^{-3})	2.035	2.090
μ (mm^{-1})	3.328	4.039
F (000)	1076	1088
Reflections collected	9883	10964
Reflections unique	7090	8147
S on F^2	1.024	1.046
R$_{int}$	0.0137	0.0158
parameters	532	532
R$_1$, wR$_2$[a][I>2σ(I)]	0.0234, 0.0608	0.0260, 0.0693
R$_1$, wR$_2$[a] (all data)	0.0270,0.0628	0.0286, 0.0708

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2=[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2. Selected bond distances /Å and bond angles /° forMOFs.

MOF-Sm			
Sm(1)-O(6)#1	2.369(2)	Sm(1)-O(2)	2.397(2)
Sm(1)-O(5)	2.406(3)	Sm(1)-O(3)#2	2.431(2)
Sm(1)-O(4)#3	2.448(2)	Sm(1)-O(1W)	2.470(3)
Sm(1)-O(1)	2.593(2)	Sm(1)-N(9)#4	2.619(3)
Sm(1)-O(3)#3	2.718(2)	Sm(2)-O(7)#5	2.369(2)
Sm(2)-O(11)#6	2.371(2)	Sm(2)-O(8)	2.407(3)
Sm(2)-O(9)	2.463(2)	Sm(2)-O(12)#3	2.481(2)
Sm(2)-O(10)	2.495(2)	Sm(2)-O(3W)	2.511(3)
Sm(2)-O(2W)	2.527(2)	Sm(2)-O(11)#3	2.669(2)
O(1)-C(1)	1.255(4)	O(2)-C(1)	1.265(4)
O(3)-C(8)	1.267(4)	O(3)-Sm(1)#2	2.431(2)
O(3)-Sm(1)#7	2.718(2)	O(4)-C(8)	1.243(4)
O(4)-Sm(1)#7	2.448(2)	O(5)-C(11)	1.260(4)
O(6)-C(11)	1.249(4)	O(6)-Sm(1)#1	2.369(2)
O(7)-C(18)	1.264(4)	O(7)-Sm(2)#5	2.369(2)
O(8)-C(18)	1.253(4)	O(9)-C(21)	1.258(4)
O(10)-C(21)	1.257(4)	O(11)-C(28)	1.272(4)
O(11)-Sm(2)#6	2.371(2)	O(11)-Sm(2)#7	2.669(2)
O(12)-C(28)	1.253(4)	O(12)-Sm(2)#7	2.481(2)
N(1)-C(9)	1.338(5)	N(1)-N(2)	1.365(4)

N(1)-C(6)	1.433(4)	N(2)-C(10)	1.318(5)
N(3)-C(9)	1.313(5)	N(3)-C(10)	1.346(6)
N(4)-C(19)	1.336(5)	N(4)-N(5)	1.345(4)
N(4)-C(16)	1.440(4)	N(5)-C(20)	1.322(5)
N(6)-C(19)	1.297(5)	N(6)-C(20)	1.342(6)
N(7)-C(30)	1.333(4)	N(7)-N(8)	1.371(4)
N(7)-C(26)	1.431(4)	N(8)-C(29)	1.306(5)
N(9)-C(30)	1.322(4)	N(9)-C(29)	1.358(5)
N(9)-Sm(1)#8	2.619(3)		
O(6)#1-Sm(1)-O(2)	140.09(9)	O(6)#1-Sm(1)-O(5)	133.48(8)
O(2)-Sm(1)-O(5)	80.73(9)	O(6)#1-Sm(1)-O(3)#2	77.50(8)
O(2)-Sm(1)-O(3)#2	101.61(8)	O(5)-Sm(1)-O(3)#2	71.44(8)
O(6)#1-Sm(1)-O(4)#3	81.34(9)	O(2)-Sm(1)-O(4)#3	125.87(8)
O(5)-Sm(1)-O(4)#3	88.90(10)	O(3)#2-Sm(1)-O(4)#3	124.98(8)
O(6)#1-Sm(1)-O(1W)	77.79(8)	O(2)-Sm(1)-O(1W)	81.35(9)
O(5)-Sm(1)-O(1W)	143.41(8)	O(3)#2-Sm(1)-O(1W)	143.79(9)
O(4)#3-Sm(1)-O(1W)	76.34(10)	O(6)#1-Sm(1)-O(1)	144.39(8)
O(2)-Sm(1)-O(1)	52.17(7)	O(5)-Sm(1)-O(1)	72.05(8)
O(3)#2-Sm(1)-O(1)	137.94(8)	O(4)#3-Sm(1)-O(1)	74.02(8)
O(1W)-Sm(1)-O(1)	71.73(8)	O(6)#1-Sm(1)-N(9)#4	71.29(9)
O(2)-Sm(1)-N(9)#4	70.43(9)	O(5)-Sm(1)-N(9)#4	127.90(10)

O(3)#2-Sm(1)-N(9)#4	73.14(9)	O(4)#3-Sm(1)-N(9)#4	143.11(11)
O(1W)-Sm(1)-N(9)#4	74.10(10)	O(1)-Sm(1)-N(9)#4	115.89(8)
O(6)#1-Sm(1)-O(3)#3	65.98(8)	O(2)-Sm(1)-O(3)#3	153.23(8)
O(5)-Sm(1)-O(3)#3	72.97(8)	O(3)#2-Sm(1)-O(3)#3	74.95(8)
O(4)#3-Sm(1)-O(3)#3	50.06(7)	O(1W)-Sm(1)-O(3)#3	117.42(8)
O(1)-Sm(1)-O(3)#3	112.91(7)	N(9)#4-Sm(1)-O(3)#3	130.85(8)
O(7)#5-Sm(2)-O(11)#6	76.16(9)	O(7)#5-Sm(2)-O(8)	134.21(9)
O(11)#6-Sm(2)-O(8)	74.76(9)	O(7)#5-Sm(2)-O(9)	144.14(9)
O(11)#6-Sm(2)-O(9)	139.63(9)	O(8)-Sm(2)-O(9)	73.26(10)
O(7)#5-Sm(2)-O(12)#3	85.39(9)	O(11)#6-Sm(2)-O(12)#3	123.79(8)
O(8)-Sm(2)-O(12)#3	82.32(10)	O(9)-Sm(2)-O(12)#3	75.19(8)
O(7)#5-Sm(2)-O(10)	144.57(8)	O(11)#6-Sm(2)-O(10)	94.70(8)
O(8)-Sm(2)-O(10)	72.57(9)	O(9)-Sm(2)-O(10)	52.37(8)
O(12)#3-Sm(2)-O(10)	126.13(8)	O(7)#5-Sm(2)-O(3W)	74.81(10)
O(11)#6-Sm(2)-O(3W)	142.84(9)	O(8)-Sm(2)-O(3W)	142.28(10)
O(9)-Sm(2)-O(3W)	71.46(11)	O(12)#3-Sm(2)-O(3W)	76.24(11)
O(10)-Sm(2)-O(3W)	95.65(11)	O(7)#5-Sm(2)-O(2W)	74.71(9)
O(11)#6-Sm(2)-O(2W)	76.73(8)	O(8)-Sm(2)-O(2W)	130.03(10)
O(9)-Sm(2)-O(2W)	106.46(9)	O(12)#3-Sm(2)-O(2W)	147.28(10)
O(10)-Sm(2)-O(2W)	69.87(8)	O(3W)-Sm(2)-O(2W)	73.63(10)
O(7)#5-Sm(2)-O(11)#3	67.42(8)	O(11)#6-Sm(2)-O(11)#3	73.55(8)

O(8)-Sm(2)-O(11)#3	70.86(9)	O(9)-Sm(2)-O(11)#3	117.10(8)
O(12)#3-Sm(2)-O(11)#3	50.42(7)	O(10)-Sm(2)-O(11)#3	143.35(9)
O(3W)-Sm(2)-O(11)#3	114.85(10)	O(2W)-Sm(2)-O(11)#3	136.16(7)
MOF-Tb			
Tb(1)-O(6)#1	2.321(2)	Tb(1)-O(2)	2.357(2)
Tb(1)-O(5)	2.370(3)	Tb(1)-O(3)#2	2.373(2)
Tb(1)-O(4)#3	2.397(2)	Tb(1)-O(1W)	2.424(3)
Tb(1)-O(1)	2.568(2)	Tb(1)-N(9)#4	2.587(3)
Tb(1)-O(3)#3	2.724(2)	Tb(2)-O(11)#5	2.322(2)
Tb(2)-O(7)#6	2.325(2)	Tb(2)-O(8)	2.365(3)
Tb(2)-O(9)	2.426(2)	Tb(2)-O(12)#3	2.436(2)
Tb(2)-O(10)	2.455(2)	Tb(2)-O(3W)	2.468(3)
Tb(2)-O(2W)	2.486(2)	Tb(2)-O(11)#3	2.661(2)
O(1)-C(1)	1.257(4)	O(2)-C(1)	1.261(4)
O(3)-C(8)	1.263(4)	O(3)-Tb(1)#2	2.374(2)
O(3)-Tb(1)#7	2.724(2)	O(4)-C(8)	1.255(4)
O(4)-Tb(1)#7	2.397(2)	O(5)-C(11)	1.264(4)
O(6)-C(11)	1.251(4)	O(6)-Tb(1)#1	2.321(2)
O(7)-C(18)	1.263(4)	O(7)-Tb(2)#6	2.325(2)
O(8)-C(18)	1.249(4)	O(9)-C(21)	1.254(4)
O(10)-C(21)	1.254(4)	O(11)-C(28)	1.272(4)

O(11)-Tb(2)#5	2.322(2)	O(11)-Tb(2)#7	2.661(2)
O(12)-C(28)	1.249(4)	O(12)-Tb(2)#7	2.436(2)
N(1)-C(9)	1.335(5)	N(1)-N(2)	1.357(4)
N(1)-C(6)	1.441(4)	N(2)-C(10)	1.319(5)
N(3)-C(9)	1.306(5)	N(3)-C(10)	1.363(6)
N(4)-C(19)	1.336(5)	N(4)-N(5)	1.352(4)
N(4)-C(16)	1.439(4)	N(5)-C(20)	1.318(6)
N(6)-C(19)	1.300(5)	N(6)-C(20)	1.358(6)
N(7)-C(30)	1.334(4)	N(7)-N(8)	1.367(4)
N(7)-C(26)	1.433(4)	N(8)-C(29)	1.305(5)
N(9)-C(30)	1.324(4)	N(9)-C(29)	1.363(5)
N(9)-Tb(1)#8	2.587(3)		
O(6)#1-Tb(1)-O(2)	140.80(9)	O(6)#1-Tb(1)-O(5)	133.51(8)
O(2)-Tb(1)-O(5)	80.16(9)	O(6)#1-Tb(1)-O(3)#2	77.79(8)
O(2)-Tb(1)-O(3)#2	101.04(8)	O(5)-Tb(1)-O(3)#2	71.78(8)
O(6)#1-Tb(1)-O(4)#3	81.23(10)	O(2)-Tb(1)-O(4)#3	126.01(8)
O(5)-Tb(1)-O(4)#3	88.13(10)	O(3)#2-Tb(1)-O(4)#3	124.84(8)
O(6)#1-Tb(1)-O(1W)	77.56(9)	O(2)-Tb(1)-O(1W)	82.08(9)
O(5)-Tb(1)-O(1W)	143.29(9)	O(3)#2-Tb(1)-O(1W)	143.58(9)
O(4)#3-Tb(1)-O(1W)	76.84(10)	O(6)#1-Tb(1)-O(1)	143.79(8)
O(2)-Tb(1)-O(1)	52.71(7)	O(5)-Tb(1)-O(1)	71.85(8)

O(3)#2-Tb(1)-O(1)	138.19(8)	O(4)#3-Tb(1)-O(1)	73.50(8)
O(1W)-Tb(1)-O(1)	71.80(9)	O(6)#1-Tb(1)-N(9)#4	71.53(9)
O(2)-Tb(1)-N(9)#4	70.82(9)	O(5)-Tb(1)-N(9)#4	128.18(10)
O(3)#2-Tb(1)-N(9)#4	72.90(9)	O(4)#3-Tb(1)-N(9)#4	143.59(11)
O(1W)-Tb(1)-N(9)#4	74.08(10)	O(1)-Tb(1)-N(9)#4	116.40(8)
O(6)#1-Tb(1)-O(3)#3	65.71(8)	O(2)-Tb(1)-O(3)#3	152.62(8)
O(5)-Tb(1)-O(3)#3	72.79(8)	O(3)#2-Tb(1)-O(3)#3	74.70(8)
O(4)#3-Tb(1)-O(3)#3	50.19(8)	O(1W)-Tb(1)-O(3)#3	117.72(8)
O(1)-Tb(1)-O(3)#3	112.79(7)	N(9)#4-Tb(1)-O(3)#3	130.48(8)
O(11)#5-Tb(2)-O(7)#6	77.10(9)	O(11)#5-Tb(2)-O(8)	75.32(9)
O(7)#6-Tb(2)-O(8)	134.35(9)	O(11)#5-Tb(2)-O(9)	139.09(9)
O(7)#6-Tb(2)-O(9)	143.55(10)	O(8)-Tb(2)-O(9)	73.79(10)
O(11)#5-Tb(2)-O(12)#3	124.52(8)	O(7)#6-Tb(2)-O(12)#3	85.37(9)
O(8)-Tb(2)-O(12)#3	81.24(11)	O(9)-Tb(2)-O(12)#3	76.00(8)
O(11)#5-Tb(2)-O(10)	92.32(8)	O(7)#6-Tb(2)-O(10)	144.17(9)
O(8)-Tb(2)-O(10)	72.61(10)	O(9)-Tb(2)-O(10)	53.06(8)
O(12)#3-Tb(2)-O(10)	127.12(8)	O(11)#5-Tb(2)-O(3W)	143.15(10)
O(7)#6-Tb(2)-O(3W)	74.27(11)	O(8)-Tb(2)-O(3W)	141.46(10)
O(9)-Tb(2)-O(3W)	70.92(11)	O(12)#3-Tb(2)-O(3W)	75.72(11)
O(10)-Tb(2)-O(3W)	97.45(12)	O(11)#5-Tb(2)-O(2W)	77.16(8)
O(7)#6-Tb(2)-O(2W)	74.06(9)	O(8)-Tb(2)-O(2W)	132.12(10)

O(9)-Tb(2)-O(2W)	105.17(9)	O(12)#3-Tb(2)-O(2W)	146.20(10)
O(10)-Tb(2)-O(2W)	70.20(9)	O(3W)-Tb(2)-O(2W)	73.06(11)
O(11)#5-Tb(2)-O(11)#3	73.96(8)	O(7)#6-Tb(2)-O(11)#3	67.21(8)
O(8)-Tb(2)-O(11)#3	70.58(9)	O(9)-Tb(2)-O(11)#3	118.73(8)
O(12)#3-Tb(2)-O(11)#3	50.82(8)	O(10)-Tb(2)-O(11)#3	142.87(9)
O(3W)-Tb(2)-O(11)#3	114.33(11)	O(2W)-Tb(2)-O(11)#3	135.65(8)

Symmetry codes:

For **MOF-Sm**: #1 (-x, -y+1, -z), #2 (-x+1, -y+1, -z), #3 (x-1, y, z), #4 (x, y, z-1), #5 (-x, -y, -z+1), #6 (-x+1, -y, -z+1), #7 (x+1 , y, z), #8 (x, y, z+1);

For **MOF-Tb**: #1 (-x, -y+1, -z), #2 (-x+1, -y+1, -z), #3 (x-1, y, z), #4 (x, y, z-1), #5 (-x+1, -y, -z+1), #6 (-x, -y, -z+1), #7 (x+1, y, z), #8 (x, y, z+1).

Table S3 The photocatalytic Degradation of Aqueous dyes byselected Ln-based MOFs

Formula	Ligand	Efficiency (%)	Light resou	refere nce

			rce	
La$_2$(adda)$_3$(H$_2$O)$_2$]	H$_2$adda= (2E,2′E)-3,3′-(anthracene-9,10-diyl) diacrylic acid	91.2 (Rh B, 120 min)	Vis	1
[Ce(H$_2$L)$_{1.5}$(H$_2$O)(DMF)]	H$_2$L= 4,4'-(diethynylanthracene-9,10-diyl)dibenzoic acid	99(MB,12 min)	vis	2
[Pr(TBDC)$_{1.5}$(H$_2$O)]	H$_2$TBDC=2,3,5,6tetramethyl-1,4-benzenedicarboxylic acid	100(CR, 24h)	xenon lamp	3
[(CH$_3$)$_2$NH$_2$]$_2$[Eu$_6$(OH)$_8$(ADBA)$_6$(H$_2$O)$_6$].	H$_2$ADBA= 4,4'-(9,10-anthracenediyl)dibenzoic acid	(MB)	vis	4
[Eu(HL)$_3$]	H$_2$L= Chalcone dicarboxylic acid ligand	44% (Rh B, 80min)	UV	5
[Gd(L)$_{1.5}$(H$_2$O)$_2$]	H$_2$L= N,N'dioxide-3,3'benzocinnoline dicarboxylic acid	81.6% (Rh B, 120min)	UV	6
[Tb(2-NCP)(AA)]	2-HNCP= 2-(2-carboxyphenyl) imidazo(4,5-f)-(1,10)phenanthroline and H$_2$AA= adipic acid	41(MB. 400)	vis	7
[(UO$_2$(pydc)(H$_2$O)]	H$_2$pydc= 2,5-pyridinedicarboxylic acid	39(Rhb, 90)	UV	8
[Yb(L^2)$_{0.5}$(NO$_3$)(DMF)$_2$]	H$_4$L^2= 5,5'-(diazene-1,2-diyl)diisophthalic acid	78%(Rh b, 120)	UV	9
[Ln$_2$(H$_2$O)$_3$(L)$_3$]	H$_2$L=5-(1H-1,2,4-triazol-1-yl)-1,3-benzenedicarboxylic acid	71.55 (MV, 40min)	UV	This work
Rh B = Rhodamine B; MB = Methylene blue ; CR= Congo red				

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