Supporting information

A series of rare-earth phosphine-oxygen complexes containing $[PW_{12}O_{40}]^{3-}$ with highly efficient photocatalytic degradation of MB

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Electronic Supplementary Information (ESI) available: crystal structure information, IR spectra, etc. CCDC 2247667-2247677. For ESI and crystallographic data in CIF or other electronic format See DOI: 10.1039/x0xx00000x

Caption of Figure

Caption of Table

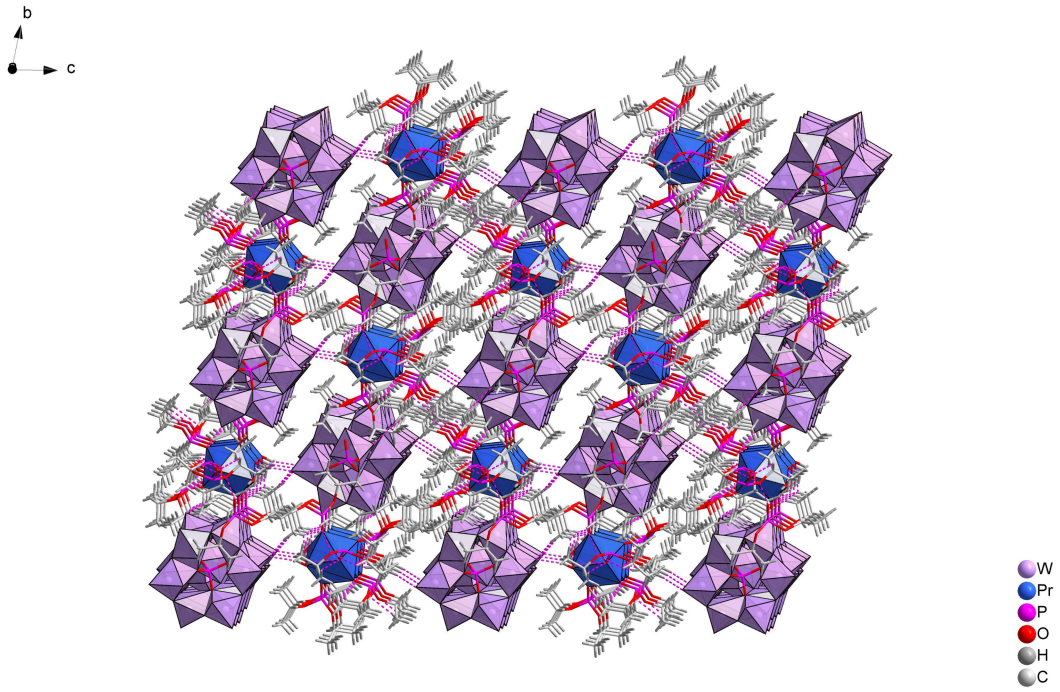

Fig. S1 Three-dimensional molecular stacking structure of complex **2**.

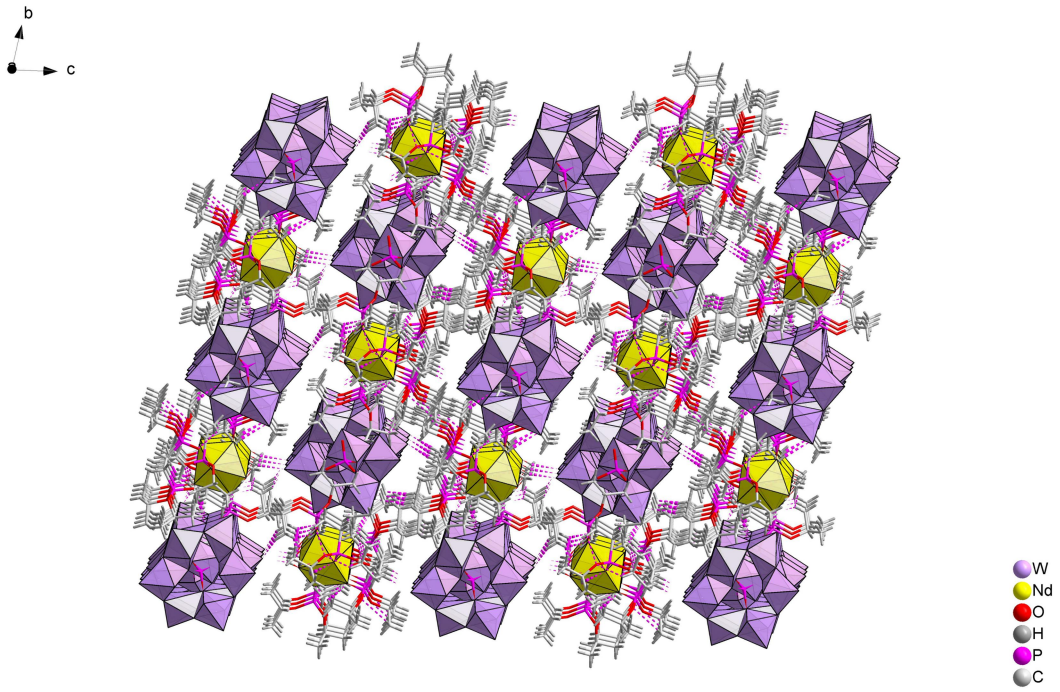

Fig. S2 Three-dimensional molecular stacking structure of complex **3**.

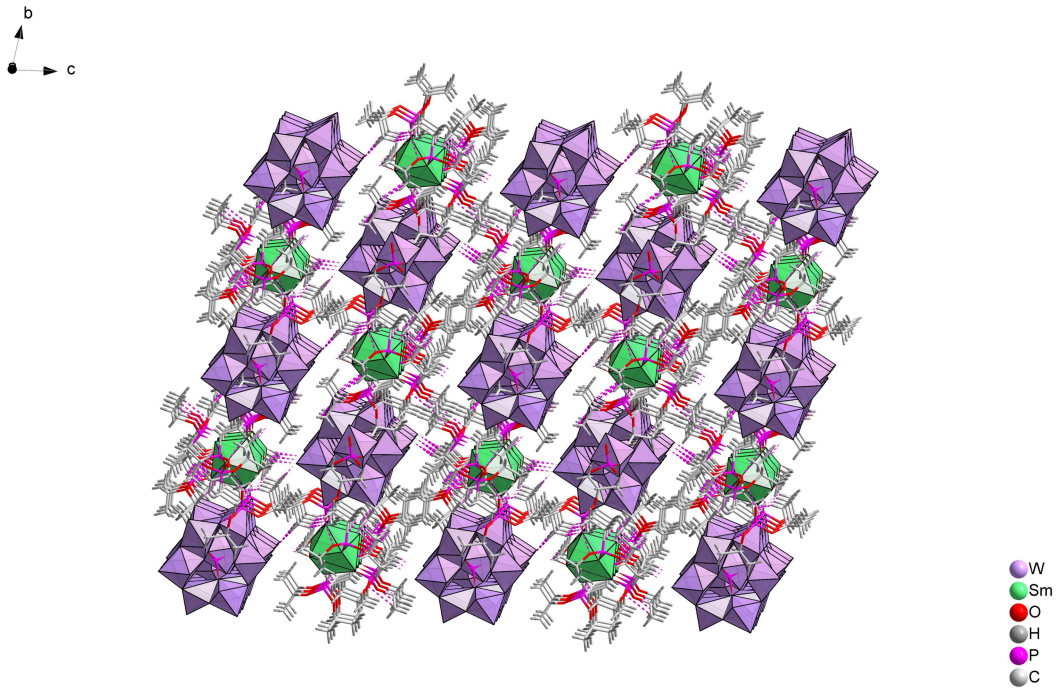

Fig. S3 Three-dimensional molecular stacking structure of complex **4**.

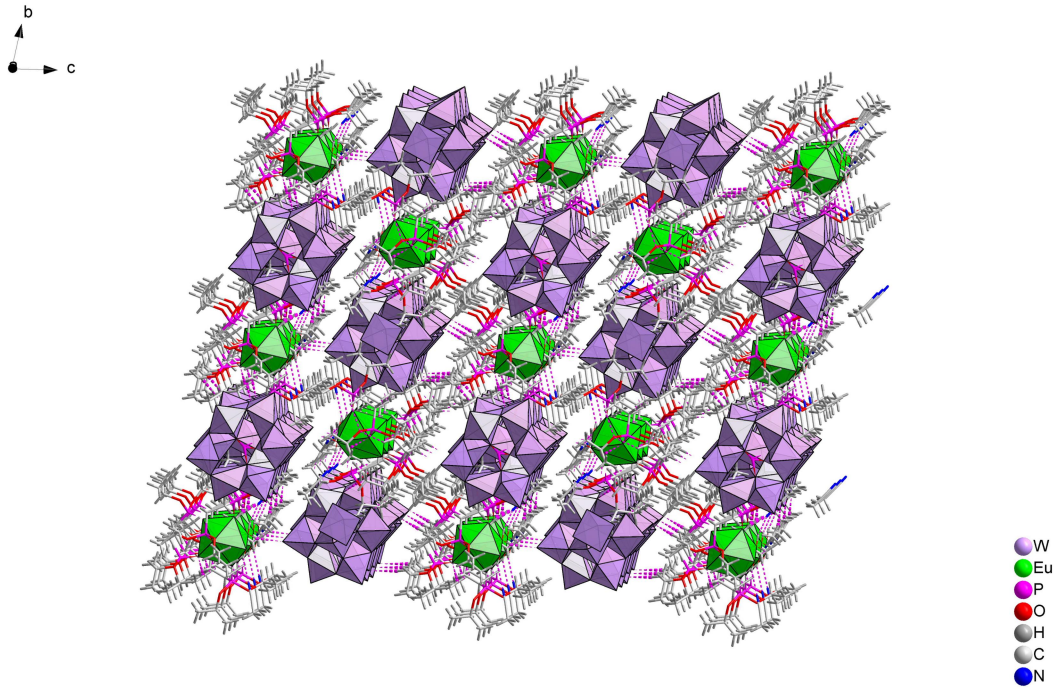

Fig. S4 Three-dimensional molecular stacking structure of complex **5**.

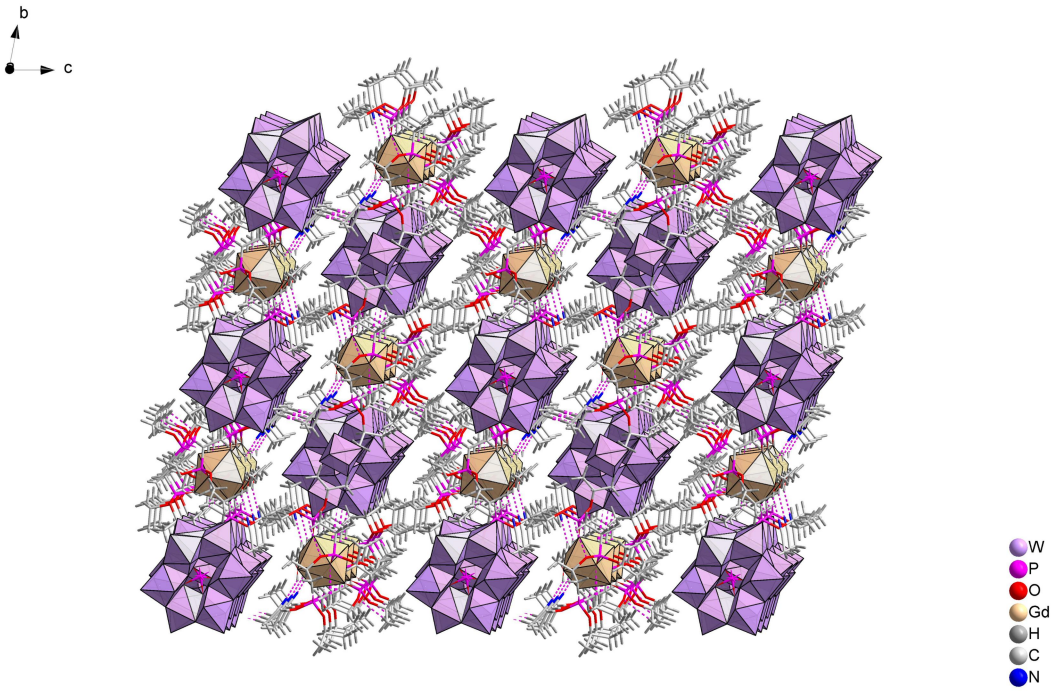

Fig. S5 Three-dimensional molecular stacking structure of complex **6**.

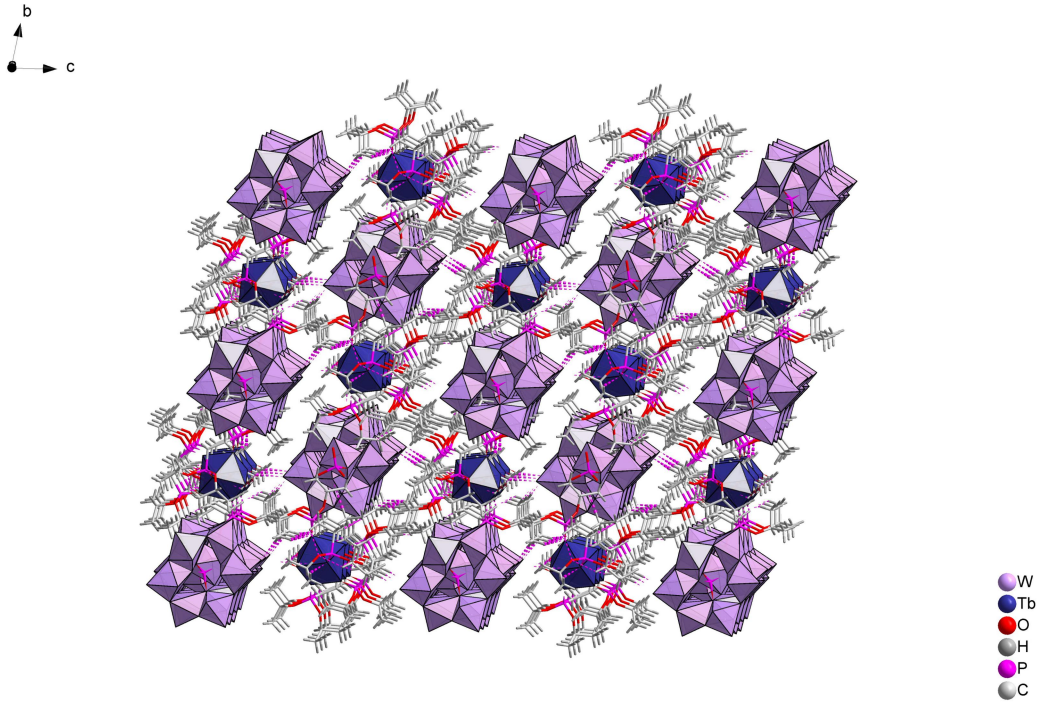

Fig. S6 Three-dimensional molecular stacking structure of complex **7**.

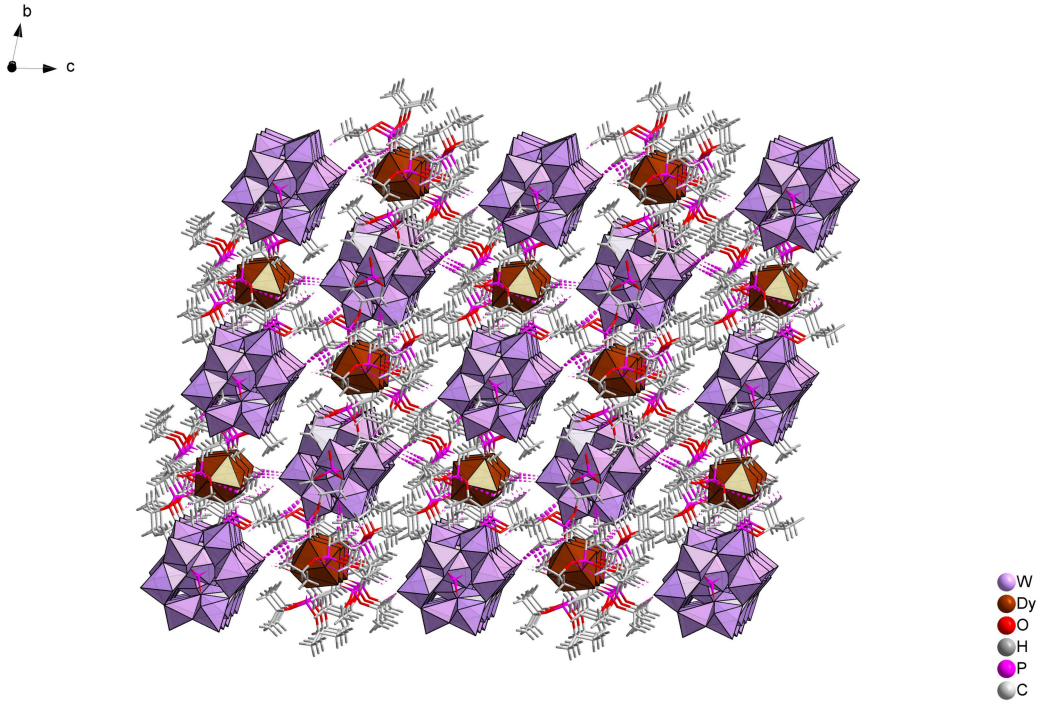

Fig. S7 Three-dimensional molecular stacking structure of complex **8**.

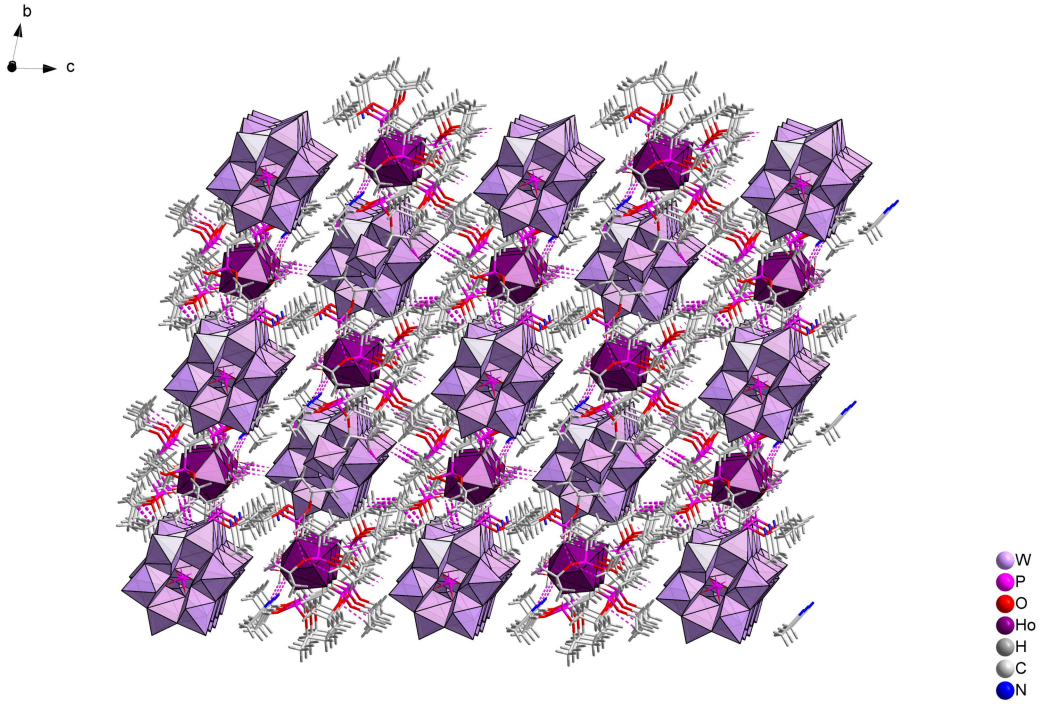

Fig. S8 Three-dimensional molecular stacking structure of complex **9**.

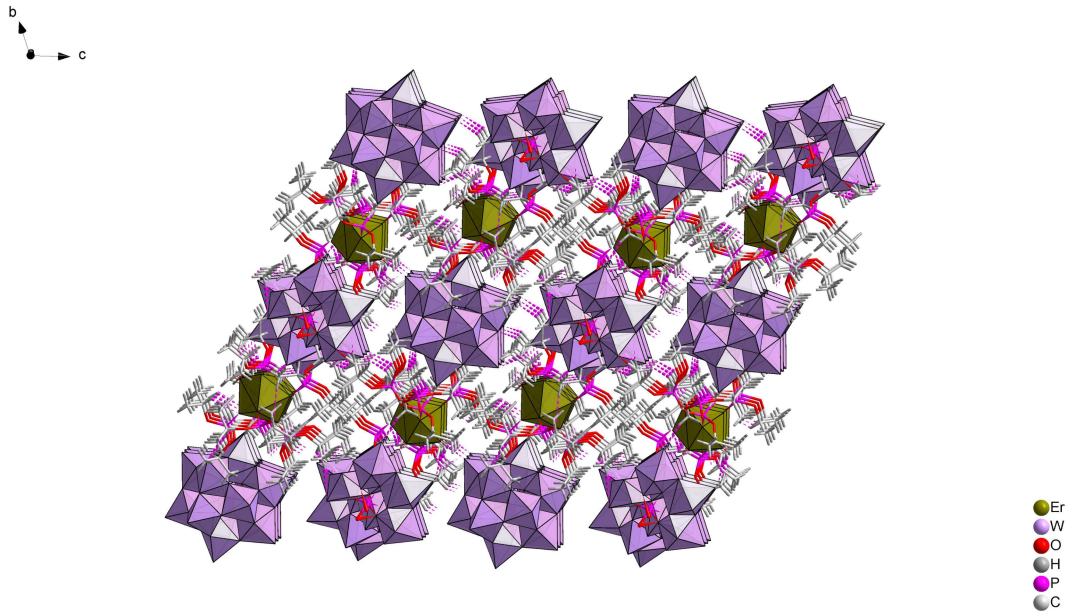

Fig. S9 Three-dimensional molecular stacking structure of complex **10**.

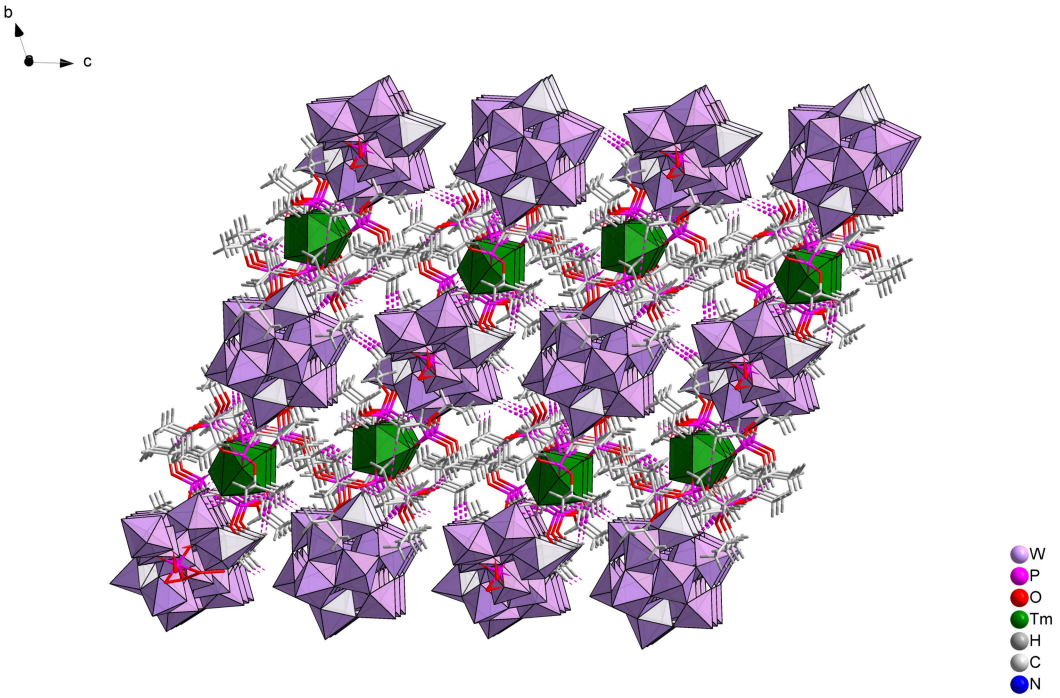

Fig. S10 Three-dimensional molecular stacking structure of complex **11**.

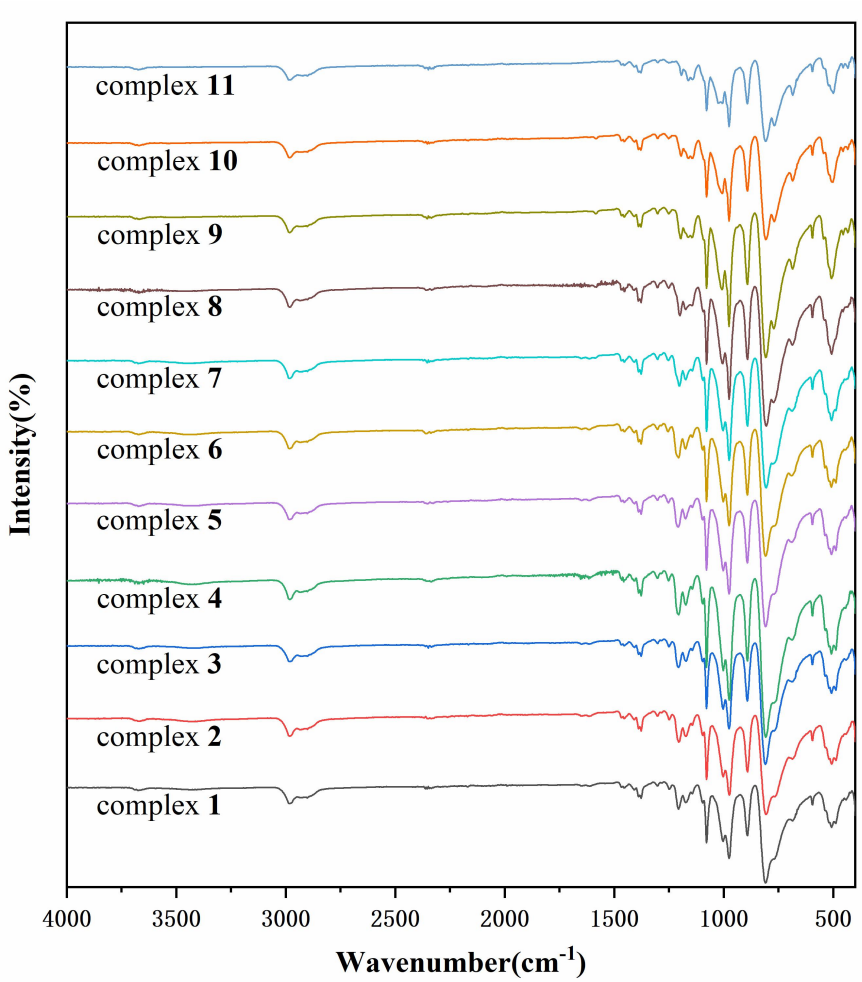

Fig. S11 Infrared spectra of complexes **1-11**.

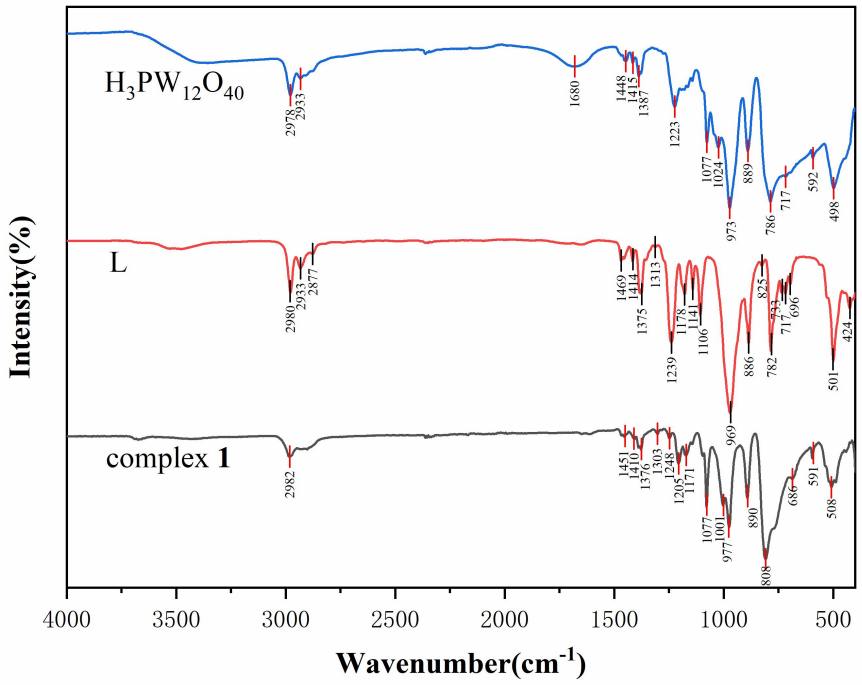

Fig. S12 Infrared spectra of complex **1**, ligand L and polyoxometalate $H_3PW_{12}O_{40}$.

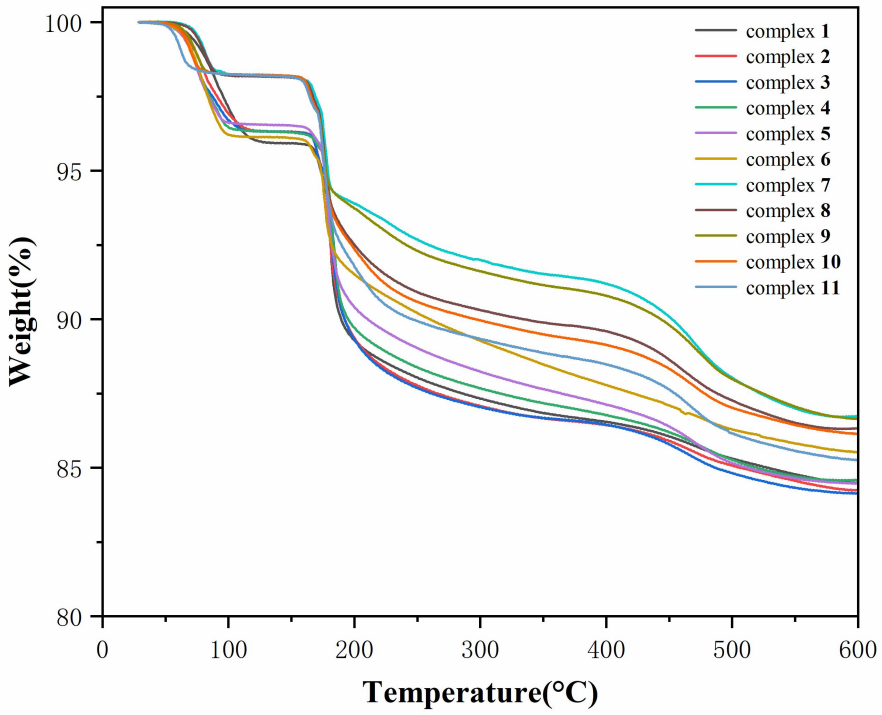

Fig. S13 Thermogravimetric curves of complexes **1-11**.

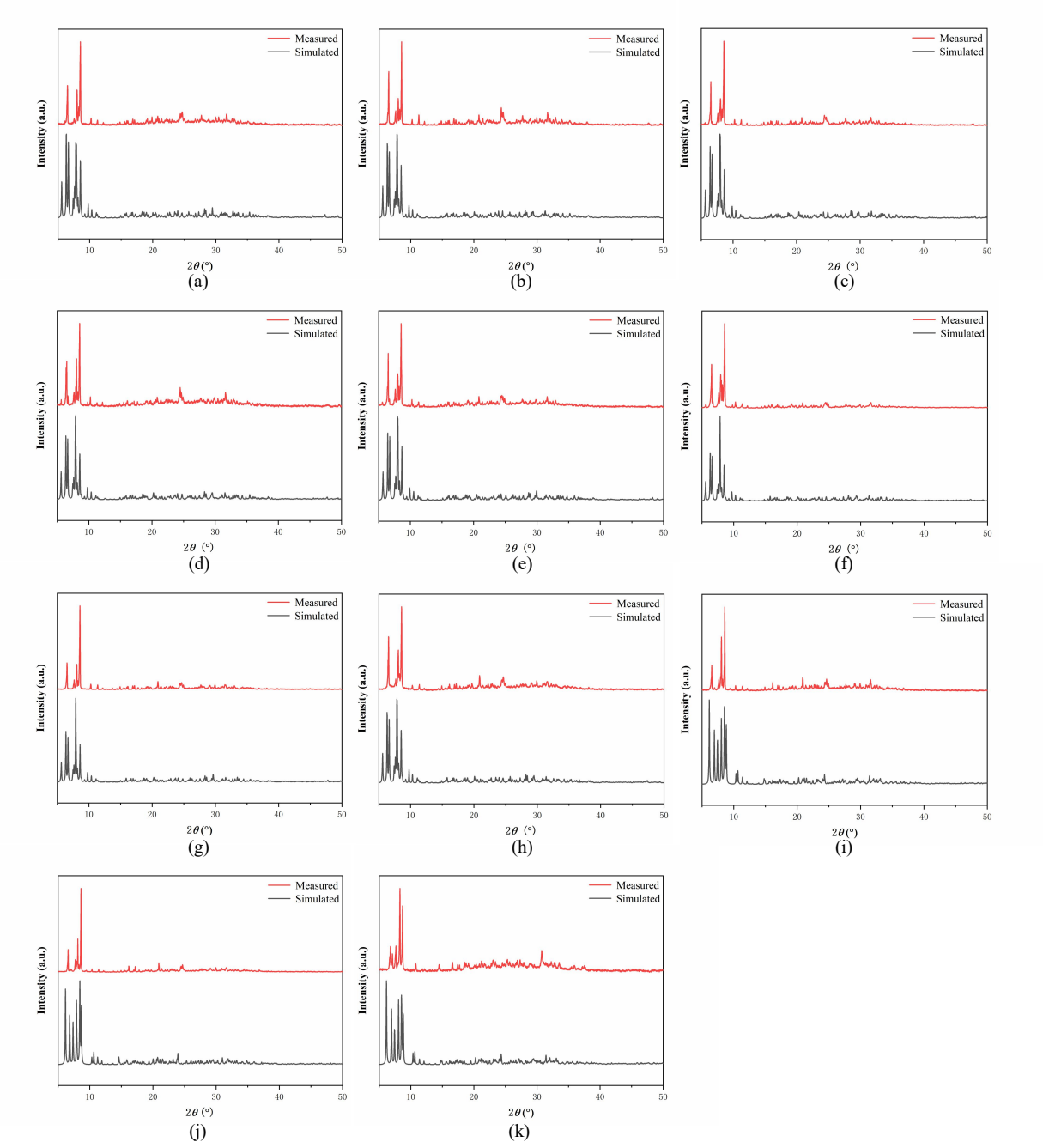

Fig. S14 Powder X-ray diffraction of complexes **1-11**.

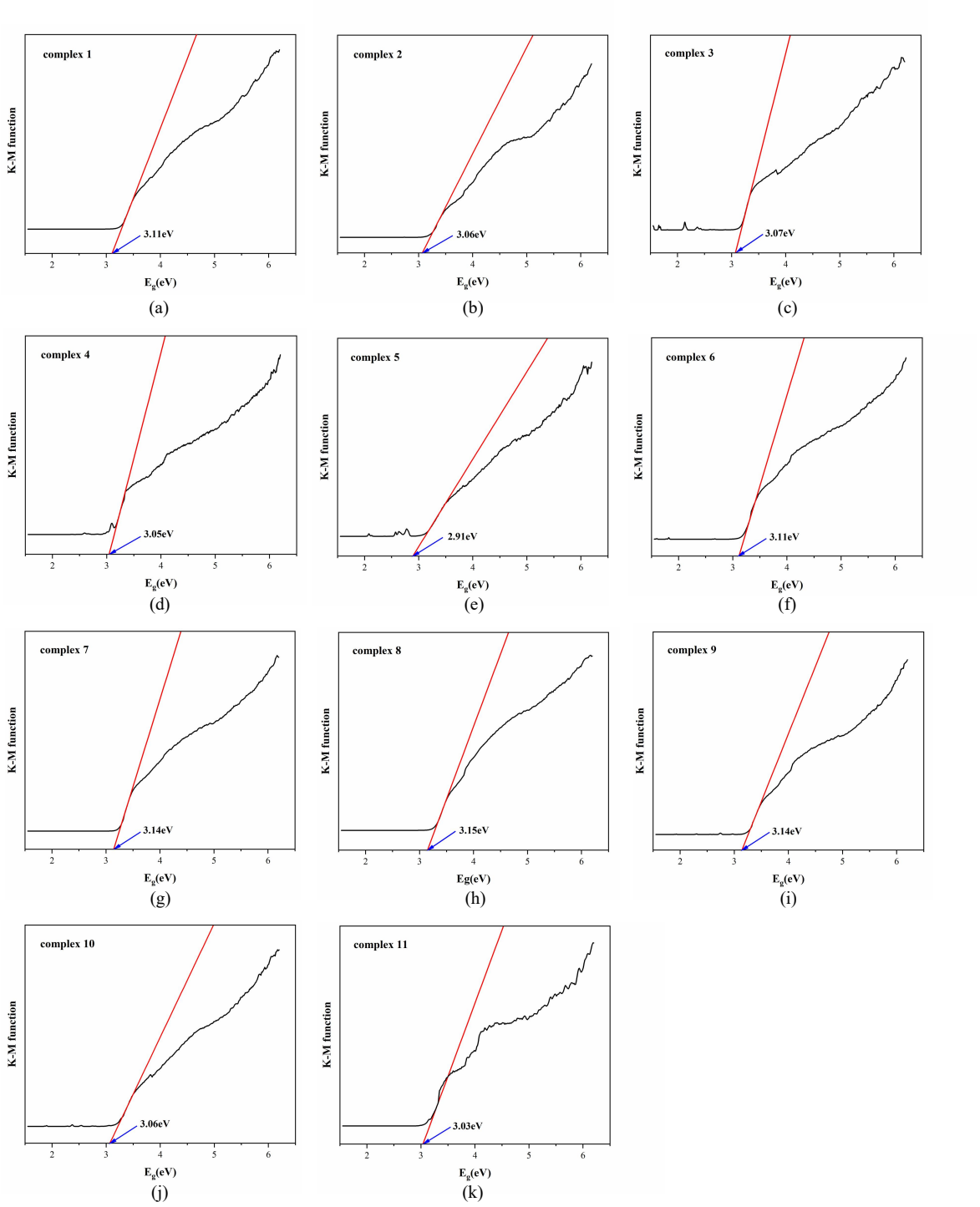

Fig. S15 Solid UV-Vis diffuse reflectance spectrum of K-M function vs Eg for complexes **1-11**.

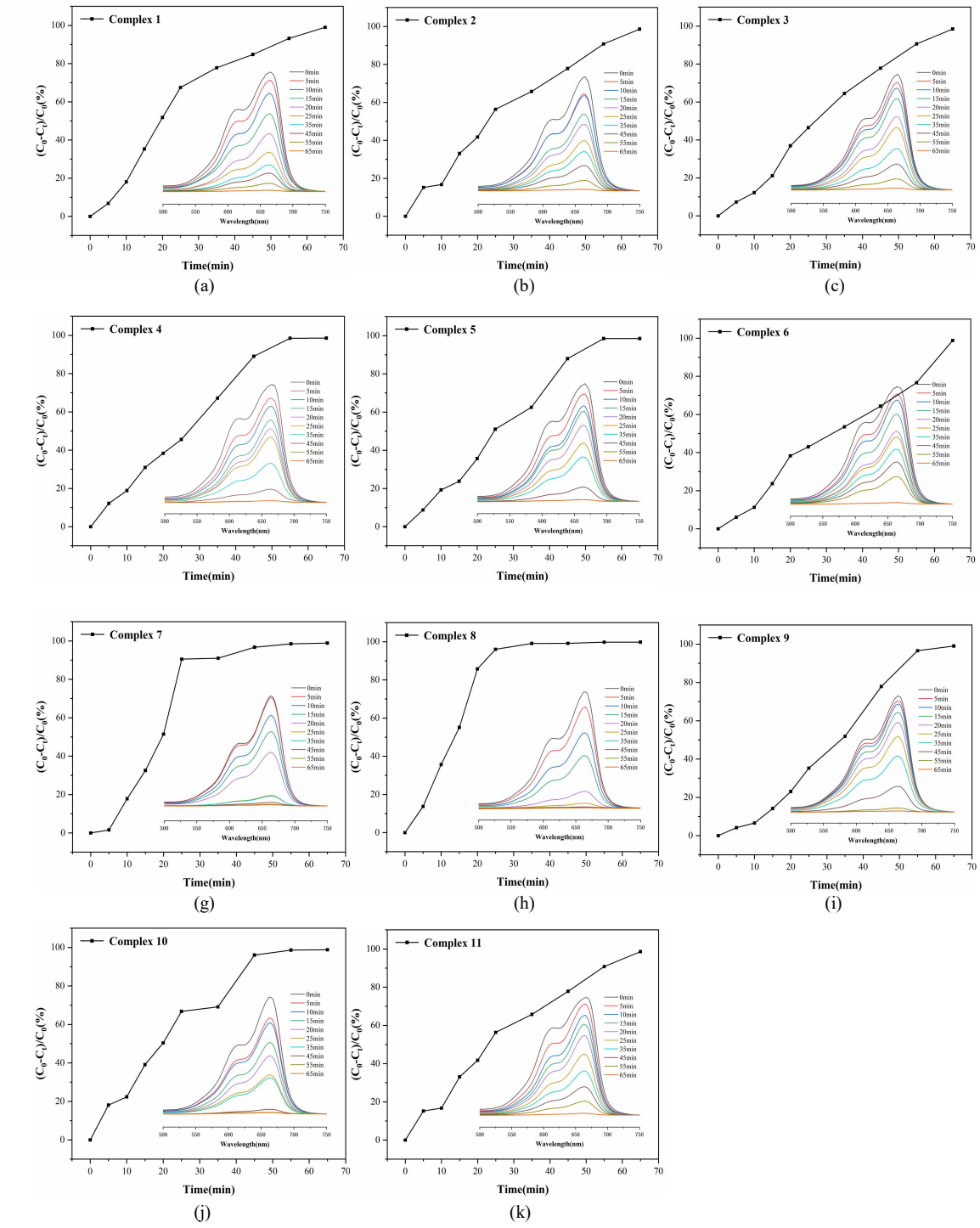

Fig. S16 UV-visible spectra (inside) and MB degradation efficiency curves (outside) for complexes **1-11**.

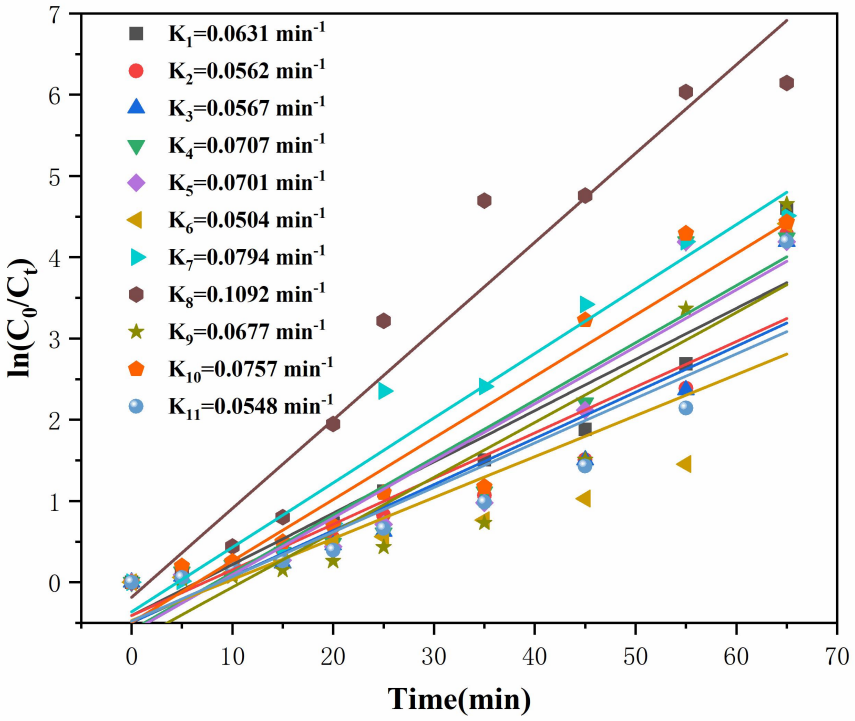

Fig. S17 Linear relationship of $\ln(C_0/C_t)$ reaction time over complexes **1–11** in degradation of MB.

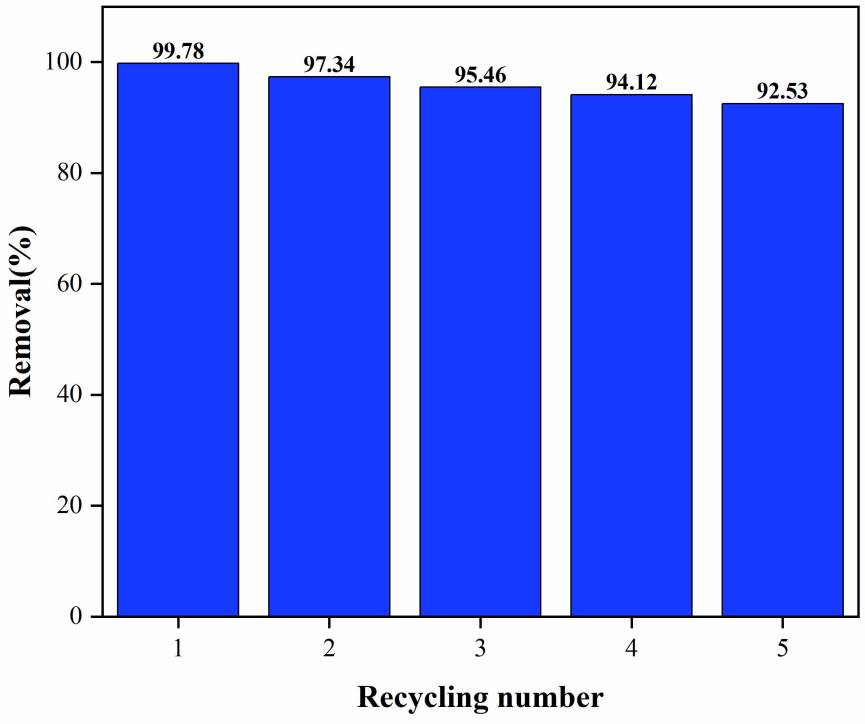

Fig. S18 Efficiency of 5 cycles photocatalytic degradation for complex **8**.

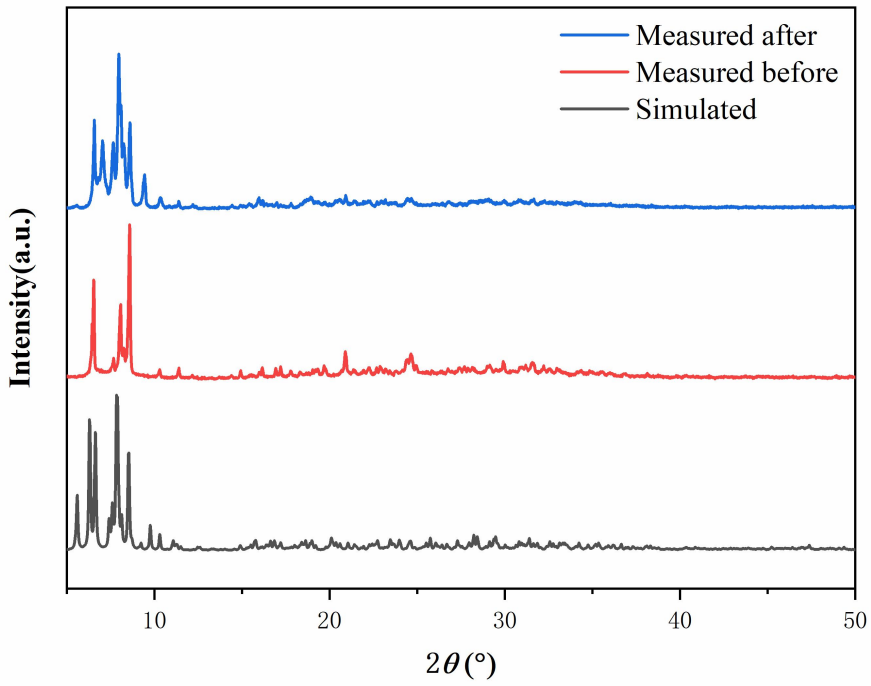

Fig. S19 Comparison of PXRD before and after catalysis of complex **8**.

Table S1 The reagents required for the experiment.

Reagent Name	Purity	Manufacturer
Lanthanum chloride salt ($LnCl_3 \cdot 6H_2O$)	99.99%	Changcheng Chemical Technology Development Co.
Tetraisopropyl ethylene diphosphonate ($C_{14}H_{32}O_4P_2$)	99.0%	Alfa Aesar (China) Chemical Co.
Phosphotungstic acid hydrate ($H_3PW_{12}O_{40} \cdot xH_2O$)	AR	Shanghai Aladdin Biochemical Technology Co.
Acetonitrile (CH_3CN)	AR	Shanghai Aladdin Biochemical Technology Co.

Table S2 The instruments required for the experiment.

Instrument Name	Model	Manufacturer
Electronic Balance	AR124CN	OHAUS Instruments (Changzhou) Co.
Intelligent Magnetic Stirrer	ZNCL-BS140	Shanghai Lingke Industrial Development Co.
X-ray single crystal diffraction instrument	D8 venture	Bruker, Germany
Elemental Analyser	Elementar Vario MICRO cube	Elementar, Germany
Fourier Infrared Spectroscopy	Bruker Vertex 70	Bruker Biotechnology Group Inc.
Thermogravimetric Analyser	TG 209 F3 Tarsus	NETZSCH, Germany
X-ray Powder Diffractometer	D8 advance	Bruker, Germany
UV-Vis Diffuse Reflection Spectrometer	Nicolet Evolution 500	Thermo Corporation, USA
Photocatalytic high	GGZ400	Shanghai Jiguang Special Lighting

pressure mercury lamp power supply		Appliance Factory
Centrifuge	TG16-WS	Hunan Xiangyi Laboratory Instrument Development Co.
UV-Vis Spectrometer	UV-2550	Shimadzu, Japan
Terahertz Time Domain Spectroscopy	self-constructed	Minzu University of China

Table S3 Crystallographic and refinement data for complexes **1-11**.

Complex	**1**	**2**	**3**	**4**
Empirical formula	$C_{42}H_{100}O_{60}P_7W_{12}$ Ce	$C_{42}H_{100}O_{60}P_7W_{12}$ Pr	$C_{42}H_{100}O_{60}P_7W_{12}$ Nd	$C_{42}H_{100}O_{60}P_7W_{12}$ Sm
Formula weight	4128.33	4129.11	4132.44	4138.55
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1
a (Å)	15.8992(14)	15.9297(18)	15.6938(15)	15.8105(16)
b (Å)	16.2547(16)	16.2805(19)	16.0627(14)	16.1724(17)
c (Å)	21.196(2)	21.296(2)	20.983(2)	21.118(2)
α (°)	78.983(2)	79.204(2)	79.328(10)	79.484(10)
β (°)	83.604(3)	83.313(3)	83.149(2)	83.225(2)
γ (°)	89.648(4)	89.273(4)	89.207(3)	89.199(3)
V (Å^3)	5342.7(9)	5388.1(11)	5160.8(8)	5271.9(9)
Z	2	2	2	2
D_{calc}(g/cm^3)	2.566	2.545	2.659	2.607
F(000)	3766	3768	3770	3774
R_{int}	0.0000	0.0841	0.0939	0.1483
R_1 [I>2σ(I)] [a]	0.0879	0.0800	0.0830	0.1095
ωR_2 [I>2σ(I)] [b]	0.2091	0.1768	0.1705	0.2415
R_1 [all data] [a]	0.1742	0.1495	0.1417	0.1814
ωR_2 [all data] [b]	0.2461	0.1989	0.1950	0.2724
Complex	**5**	**6**	**7**	**8**
Empirical formula	$C_{50}H_{112}O_{60}N_4P_7W_{12}$Eu	$C_{42}H_{100}O_{60}P_7W_{12}$ Gd	$C_{42}H_{100}O_{60}P_7W_{12}$ Tb	$C_{42}H_{100}O_{60}P_7W_{12}$ Dy
Formula weight	4304.38	4145.45	4147.12	4150.70
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1
a (Å)	15.6853(11)	15.9020(16)	15.7502(18)	15.8884(16)
b (Å)	15.9941(12)	16.2959(18)	16.1810(17)	16.2671(17)

c (Å)	20.9417(15)	21.296(2)	21.056(3)	21.247(2)
α (°)	79.0320(10)	79.254(2)	79.203(2)	78.978(3)
β (°)	83.155(2)	83.242(3)	83.359(3)	83.287(4)
γ (°)	88.969(2)	88.856(3)	88.955(4)	89.249(4)
V (Å^3)	5120.9(6)	5384.1(10)	5235.7(10)	5352.9(9)
Z	2	2	2	2
D_{calc}(g/cm^3)	2.792	2.557	2.631	2.575
F(000)	3952	3778	3780	3782
R_{int}	0.1015	0.0763	0.1401	0.3422
R_1 [I>2σ(I)] [a]	0.0773	0.0795	0.1018	0.1466
ωR_2 [I>2σ(I)] [b]	0.1944	0.1811	0.2291	0.3014
R_1 [all data] [a]	0.0854	0.1418	0.1799	0.2609
ωR_2 [all data] [b]	0.1985	0.1994	0.2516	0.3322
Complex	**9**	**10**	**11**	
Empirical formula	$C_{50}H_{112}O_{60}N_4P_7W_{12}Ho$	$C_{42}H_{100}O_{60}P_7W_{12}Er$	$C_{46}H_{106}O_{60}N_2P_7W_{12}Tm$	
Formula weight	4317.35	4155.46	4239.24	
Crystal system	Triclinic	Triclinic	Triclinic	
Space group	P-1	P-1	P-1	
a (Å)	15.6393(8)	15.7600(17)	15.5807(3)	
b (Å)	15.9692(8)	16.9001(18)	16.9400(3)	
c (Å)	20.8803(10)	22.290(2)	21.7710(4)	
α (°)	79.029(2)	104.230(4)	104.785(2)	
β (°)	83.166(2)	95.080(3)	94.446(3)	
γ (°)	88.783(2)	116.550(5)	116.285(4)	
V (Å^3)	5083.1(4)	5011.3(10)	4859.7(2)	
Z	2	2	2	
D_{calc}(g/cm^3)	2.821	2.754	2.897	
F(000)	3960	3786	3876	
R_{int}	0.0896	0.2524	0.0506	
R_1 [I>2σ(I)] [a]	0.0790	0.1304	0.0461	
ωR_2 [I>2σ(I)] [b]	0.1796	0.2903	0.0988	
R_1 [all data] [a]	0.0849	0.2340	0.0572	
ωR_2 [all data] [b]	0.1834	0.3450	0.1024	

[a] $R = \sum(||F_0|-|F_c||)/\sum|F_0|$.

[b] $\omega R = [\sum\omega(|F_0|^2-|F_c|^2)^2/\sum\omega|F_0|^2]^{1/2}$.

Table S4 The major bond lengths(Å) and bond angles(°) for complexes **1-11**.

1					
Ce(1)-O(41)	2.48(4)	Ce(1)-O(44)	2.51(4)	Ce(1)-O(47)	2.45(4)
Ce(1)-O(50)	2.46(3)	Ce(1)-O(53)	2.55(4)	Ce(1)-O(56)	2.55(4)

Ce(1)-O(59)	2.55(4)	Ce(1)-O(60)	2.63(4)		
O(41)-Ce(1)-O(44)	78.1(13)	O(41)-Ce(1)-O(53)	77.1(13)	O(41)-Ce(1)-O(56)	73.3(13)
O(41)-Ce(1)-O(59)	117.1(13)	O(41)-Ce(1)-O(60)	141.2(12)	O(44)-Ce(1)-O(53)	76.8(13)
O(44)-Ce(1)-O(56)	144.9(13)	O(44)-Ce(1)-O(59)	139.9(12)	O(44)-Ce(1)-O(60)	120.2(13)
O(47)-Ce(1)-O(41)	78.9(12)	O(47)-Ce(1)-O(44)	71.7(14)	O(47)-Ce(1)-O(50)	74.5(12)
O(47)-Ce(1)-O(53)	143.6(14)	O(47)-Ce(1)-O(56)	120.7(13)	O(47)-Ce(1)-O(59)	75.2(14)
O(47)-Ce(1)-O(60)	137.5(13)	O(50)-Ce(1)-O(41)	146.4(13)	O(50)-Ce(1)-O(44)	74.3(14)
O(50)-Ce(1)-O(53)	114.0(13)	O(50)-Ce(1)-O(56)	138.8(14)	O(50)-Ce(1)-O(59)	75.4(13)
O(50)-Ce(1)-O(60)	71.1(12)	O(53)-Ce(1)-O(56)	77.5(13)	O(53)-Ce(1)-O(59)	140.7(13)
O(53)-Ce(1)-O(60)	75.0(13)	O(56)-Ce(1)-O(60)	74.7(11)	O(59)-Ce(1)-O(56)	73.0(13)
O(59)-Ce(1)-O(60)	72.6(13)				
2					
Pr(1)-O(41)	2.469(3)	Pr(1)-O(44)	2.458(3)	Pr(1)-O(47)	2.453(4)
Pr(1)-O(50)	2.432(3)	Pr(1)-O(53)	2.428(3)	Pr(1)-O(56)	2.475(4)
Pr(1)-O(59)	2.496(4)	Pr(1)-O(60)	2.593(3)		
O(41)-Pr(1)-O(56)	70.82(9)	O(41)-Pr(1)-O(59)	113.46(13)	O(41)-Pr(1)-O(60)	141.30(15)
O(44)-Pr(1)-O(41)	80.29(10)	O(44)-Pr(1)-O(56)	142.98(14)	O(44)-Pr(1)-O(59)	142.91(15)
O(44)-Pr(1)-O(60)	119.13(13)	O(47)-Pr(1)-O(41)	75.61(9)	O(47)-Pr(1)-O(44)	77.01(10)
O(47)-Pr(1)-O(56)	115.91(13)	O(47)-Pr(1)-O(59)	73.89(9)	O(47)-Pr(1)-O(60)	138.29(14)
O(50)-Pr(1)-O(41)	148.66(15)	O(50)-Pr(1)-O(44)	75.55(10)	O(50)-Pr(1)-O(47)	79.71(10)
O(50)-Pr(1)-O(56)	138.76(14)	O(50)-Pr(1)-O(59)	77.05(9)	O(50)-Pr(1)-O(60)	69.37(8)
O(53)-Pr(1)-O(41)	80.57(10)	O(53)-Pr(1)-O(44)	76.72(10)	O(53)-Pr(1)-O(47)	147.00(15)
O(53)-Pr(1)-O(50)	112.31(13)	O(53)-Pr(1)-O(56)	76.13(10)	O(53)-Pr(1)-O(59)	137.62(15)
O(53)-Pr(1)-O(60)	73.06(9)	O(56)-Pr(1)-O(59)	72.08(9)	O(56)-Pr(1)-O(60)	75.63(9)
O(59)-Pr(1)-O(60)	72.45(9)				
3					
Nd(1)-O(41)	2.41(2)	Nd(1)-O(44)	2.429(19)	Nd(1)-O(47)	2.41(2)
Nd(1)-O(50)	2.36(2)	Nd(1)-O(53)	2.38(2)	Nd(1)-O(56)	2.41(2)
Nd(1)-O(59)	2.515(19)	Nd(1)-O(60)	2.55(2)		
O(41)-Nd(1)-O(44)	79.5(7)	O(41)-Nd(1)-O(59)	114.1(7)	O(41)-Nd(1)-O(60)	140.3(7)
O(44)-Nd(1)-O(59)	142.8(7)	O(44)-Nd(1)-O(60)	120.3(7)	O(47)-Nd(1)-O(41)	76.4(7)
O(47)-Nd(1)-O(44)	76.5(7)	O(47)-Nd(1)-O(59)	73.9(7)	O(47)-Nd(1)-O(60)	138.5(7)
O(50)-Nd(1)-O(41)	149.4(7)	O(50)-Nd(1)-O(44)	76.8(7)	O(50)-Nd(1)-O(47)	79.4(7)
O(50)-Nd(1)-O(53)	112.4(7)	O(50)-Nd(1)-O(56)	137.1(6)	O(50)-Nd(1)-O(59)	76.2(7)
O(50)-Nd(1)-O(60)	69.7(7)	O(53)-Nd(1)-O(41)	80.1(7)	O(53)-Nd(1)-O(44)	76.6(7)

O(53)-Nd(1)-O(47)	146.9(7)	O(53)-Nd(1)-O(56)	77.0(7)	O(53)-Nd(1)-O(59)	137.9(7)
O(53)-Nd(1)-O(60)	72.9(7)	O(56)-Nd(1)-O(41)	71.6(7)	O(56)-Nd(1)-O(44)	143.6(7)
O(56)-Nd(1)-O(47)	116.2(7)	O(56)-Nd(1)-O(59)	71.4(7)	O(56)-Nd(1)-O(60)	74.3(7)
O(59)-Nd(1)-O(60)	72.4(7)				
4					
Sm(1)-O(41)	2.39(3)	Sm(1)-O(44)	2.42(3)	Sm(1)-O(47)	2.36(3)
Sm(1)-O(50)	2.36(3)	Sm(1)-O(53)	2.34(3)	Sm(1)-O(56)	2.39(3)
Sm(1)-O(59)	2.52(2)	Sm(1)-O(60)	2.55(3)		
O(41)-Sm(1)-O(44)	79.7(9)	O(41)-Sm(1)-O(56)	71.9(9)	O(41)-Sm(1)-O(59)	115.0(9)
O(41)-Sm(1)-O(60)	141.6(9)	O(44)-Sm(1)-O(59)	141.9(9)	O(44)-Sm(1)-O(60)	118.2(10)
O(47)-Sm(1)-O(41)	77.8(10)	O(47)-Sm(1)-O(44)	77.6(9)	O(47)-Sm(1)-O(50)	79.8(10)
O(47)-Sm(1)-O(56)	115.5(9)	O(47)-Sm(1)-O(59)	72.2(8)	O(47)-Sm(1)-O(60)	136.7(10)
O(50)-Sm(1)-O(41)	149.7(9)	O(50)-Sm(1)-O(44)	75.9(9)	O(50)-Sm(1)-O(56)	137.0(9)
O(50)-Sm(1)-O(59)	76.3(9)	O(50)-Sm(1)-O(60)	67.5(9)	O(53)-Sm(1)-O(41)	77.3(9)
O(53)-Sm(1)-O(44)	75.3(9)	O(53)-Sm(1)-O(47)	145.9(9)	O(53)-Sm(1)-O(50)	112.8(9)
O(53)-Sm(1)-O(56)	77.8(9)	O(53)-Sm(1)-O(59)	140.3(8)	O(53)-Sm(1)-O(60)	75.5(10)
O(56)-Sm(1)-O(44)	144.4(9)	O(56)-Sm(1)-O(59)	71.6(9)	O(56)-Sm(1)-O(60)	76.2(10)
O(59)-Sm(1)-O(60)	73.1(9)				
5					
Eu(1)-O(45)	2.366(12)	Eu(1)-O(48)	2.426(12)	Eu(1)-O(51)	2.350(13)
Eu(1)-O(54)	2.375(12)	Eu(1)-O(57)	2.390(13)	Eu(1)-O(60)	2.393(13)
Eu(1)-O(63)	2.486(12)	Eu(1)-O(64)	2.447(14)		
O(45)-Eu(1)-O(48)	76.2(4)	O(45)-Eu(1)-O(54)	137.3(4)	O(45)-Eu(1)-O(57)	150.2(4)
O(45)-Eu(1)-O(60)	81.0(4)	O(45)-Eu(1)-O(63)	69.2(4)	O(45)-Eu(1)-O(64)	76.1(5)
O(48)-Eu(1)-O(63)	121.5(4)	O(48)-Eu(1)-O(64)	141.0(5)	O(51)-Eu(1)-O(45)	110.7(5)
O(51)-Eu(1)-O(48)	76.2(4)	O(51)-Eu(1)-O(54)	77.7(4)	O(51)-Eu(1)-O(57)	80.2(5)
O(51)-Eu(1)-O(60)	146.7(5)	O(51)-Eu(1)-O(63)	74.1(5)	O(51)-Eu(1)-O(64)	139.9(5)
O(54)-Eu(1)-O(48)	143.8(4)	O(54)-Eu(1)-O(57)	71.2(4)	O(54)-Eu(1)-O(60)	115.5(4)
O(54)-Eu(1)-O(63)	73.8(4)	O(54)-Eu(1)-O(64)	72.8(5)	O(57)-Eu(1)-O(48)	79.9(4)
O(57)-Eu(1)-O(60)	76.3(5)	O(57)-Eu(1)-O(63)	140.0(5)	O(57)-Eu(1)-O(64)	114.2(5)
O(60)-Eu(1)-O(48)	76.7(4)	O(60)-Eu(1)-O(63)	137.8(4)	O(60)-Eu(1)-O(64)	72.4(5)
O(64)-Eu(1)-O(63)	72.0(5)				
6					
Gd(1)-O(41)	2.360(16)	Gd(1)-O(44)	2.419(15)	Gd(1)-O(47)	2.392(16)

Gd(1)-O(50)	2.389(16)	Gd(1)-O(53)	2.381(16)	Gd(1)-O(56)	2.409(15)
Gd(1)-O(59)	2.478(15)	Gd(1)-O(60)	2.513(15)		
O(41)-Gd(1)-O(44)	80.3(5)	O(41)-Gd(1)-O(47)	76.4(6)	O(41)-Gd(1)-O(50)	149.1(5)
O(41)-Gd(1)-O(53)	80.7(6)	O(41)-Gd(1)-O(56)	71.4(5)	O(41)-Gd(1)-O(59)	114.3(6)
O(41)-Gd(1)-O(60)	141.6(5)	O(44)-Gd(1)-O(59)	140.6(5)	O(44)-Gd(1)-O(60)	119.7(5)
O(47)-Gd(1)-O(44)	77.6(5)	O(47)-Gd(1)-O(56)	114.9(5)	O(47)-Gd(1)-O(59)	71.4(6)
O(47)-Gd(1)-O(60)	136.7(6)	O(50)-Gd(1)-O(44)	75.2(5)	O(50)-Gd(1)-O(47)	80.1(6)
O(50)-Gd(1)-O(56)	137.9(5)	O(50)-Gd(1)-O(59)	76.0(5)	O(50)-Gd(1)-O(60)	68.6(5)
O(53)-Gd(1)-O(44)	75.5(5)	O(53)-Gd(1)-O(47)	147.1(5)	O(53)-Gd(1)-O(50)	110.4(6)
O(53)-Gd(1)-O(56)	78.8(5)	O(53)-Gd(1)-O(59)	140.6(5)	O(53)-Gd(1)-O(60)	74.2(5)
O(56)-Gd(1)-O(44)	144.3(5)	O(56)-Gd(1)-O(59)	72.9(5)	O(56)-Gd(1)-O(60)	75.4(5)
O(59)-Gd(1)-O(60)	72.5(6)				
7					
Tb(1)-O(41)	2.37(2)	Tb(1)-O(44)	2.40(2)	Tb(1)-O(47)	2.33(2)
Tb(1)-O(50)	2.36(2)	Tb(1)-O(53)	2.31(2)	Tb(1)-O(56)	2.36(2)
Tb(1)-O(59)	2.406(19)	Tb(1)-O(60)	2.48(2)		
O(41)-Tb(1)-O(44)	81.0(8)	O(41)-Tb(1)-O(59)	115.0(7)	O(41)-Tb(1)-O(60)	141.0(7)
O(44)-Tb(1)-O(59)	142.4(7)	O(44)-Tb(1)-O(60)	119.0(8)	O(47)-Tb(1)-O(41)	76.0(8)
O(47)-Tb(1)-O(44)	78.8(7)	O(47)-Tb(1)-O(50)	79.5(8)	O(47)-Tb(1)-O(56)	114.5(8)
O(47)-Tb(1)-O(59)	73.2(8)	O(47)-Tb(1)-O(60)	137.3(8)	O(50)-Tb(1)-O(41)	148.9(8)
O(50)-Tb(1)-O(44)	75.6(8)	O(50)-Tb(1)-O(56)	137.8(7)	O(50)-Tb(1)-O(59)	75.0(6)
O(50)-Tb(1)-O(60)	69.6(7)	O(53)-Tb(1)-O(41)	80.5(8)	O(53)-Tb(1)-O(44)	75.6(7)
O(53)-Tb(1)-O(47)	147.5(8)	O(53)-Tb(1)-O(50)	112.5(8)	O(53)-Tb(1)-O(56)	77.7(7)
O(53)-Tb(1)-O(59)	138.1(8)	O(53)-Tb(1)-O(60)	73.7(7)	O(56)-Tb(1)-O(41)	71.1(7)
O(56)-Tb(1)-O(44)	144.0(7)	O(56)-Tb(1)-O(59)	72.2(6)	O(56)-Tb(1)-O(60)	75.1(7)
O(59)-Tb(1)-O(60)	70.9(8)				
8					
Dy(1)-O(41)	2.43(4)	Dy(1)-O(44)	2.32(3)	Dy(1)-O(47)	2.35(4)
Dy(1)-O(50)	2.38(3)	Dy(1)-O(53)	2.28(3)	Dy(1)-O(56)	2.33(3)
Dy(1)-O(59)	2.59(3)	Dy(1)-O(60)	2.56(4)		
O(41)-Dy(1)-O(59)	114.8(10)	O(41)-Dy(1)-O(60)	140.7(11)	O(44)-Dy(1)-O(41)	79.5(11)
O(44)-Dy(1)-O(47)	78.7(12)	O(44)-Dy(1)-O(50)	75.2(12)	O(44)-Dy(1)-O(56)	143.5(12)
O(44)-Dy(1)-O(59)	143.9(10)	O(44)-Dy(1)-O(60)	117.5(12)	O(47)-Dy(1)-O(41)	72.0(12)
O(47)-Dy(1)-O(50)	81.7(12)	O(47)-Dy(1)-O(59)	75.4(12)	O(47)-Dy(1)-O(60)	142.8(11)

O(50)-Dy(1)-O(41)	146.5(13)	O(50)-Dy(1)-O(59)	76.6(9)	O(50)-Dy(1)-O(60)	71.8(11)
O(53)-Dy(1)-O(41)	80.5(12)	O(53)-Dy(1)-O(44)	72.6(12)	O(53)-Dy(1)-O(47)	143.2(12)
O(53)-Dy(1)-O(50)	111.7(12)	O(53)-Dy(1)-O(56)	80.3(11)	O(53)-Dy(1)-O(59)	139.9(11)
O(53)-Dy(1)-O(60)	72.7(12)	O(56)-Dy(1)-O(41)	72.1(12)	O(56)-Dy(1)-O(47)	112.5(11)
O(56)-Dy(1)-O(50)	139.1(12)	O(56)-Dy(1)-O(59)	71.0(9)	O(56)-Dy(1)-O(60)	75.4(11)
O(60)-Dy(1)-O(59)	73.4(12)				
9					
Ho(1)-O(41)	2.311(5)	Ho(1)-O(44)	2.326(6)	Ho(1)-O(47)	2.377(6)
Ho(1)-O(50)	2.321(6)	Ho(1)-O(53)	2.302(6)	Ho(1)-O(56)	2.341(6)
Ho(1)-O(59)	2.432(6)	Ho(1)-O(60)	2.408(7)		
O(41)-Ho(1)-O(44)	81.2(2)	O(41)-Ho(1)-O(47)	76.0(2)	O(41)-Ho(1)-O(50)	150.7(2)
O(41)-Ho(1)-O(56)	136.93(19)	O(41)-Ho(1)-O(59)	69.0(2)	O(41)-Ho(1)-O(60)	75.5(2)
O(44)-Ho(1)-O(47)	76.0(2)	O(44)-Ho(1)-O(56)	116.1(2)	O(44)-Ho(1)-O(59)	138.3(2)
O(44)-Ho(1)-O(60)	72.4(2)	O(47)-Ho(1)-O(59)	121.3(2)	O(47)-Ho(1)-O(60)	140.0(2)
O(50)-Ho(1)-O(44)	76.5(2)	O(50)-Ho(1)-O(47)	80.3(2)	O(50)-Ho(1)-O(56)	71.1(2)
O(50)-Ho(1)-O(59)	139.6(2)	O(50)-Ho(1)-O(60)	114.5(2)	O(53)-Ho(1)-O(41)	110.0(2)
O(53)-Ho(1)-O(44)	146.0(2)	O(53)-Ho(1)-O(47)	76.0(2)	O(53)-Ho(1)-O(50)	80.2(2)
O(53)-Ho(1)-O(56)	78.2(2)	O(53)-Ho(1)-O(59)	73.9(2)	O(53)-Ho(1)-O(60)	140.8(2)
O(56)-Ho(1)-O(47)	144.1(2)	O(56)-Ho(1)-O(59)	73.5(2)	O(56)-Ho(1)-O(60)	73.6(2)
O(60)-Ho(1)-O(59)	72.4(2)				
10					
Er(1)-O(41)	2.27(3)	Er(1)-O(44)	2.35(3)	Er(1)-O(47)	2.36(3)
Er(1)-O(50)	2.36(3)	Er(1)-O(53)	2.44(2)	Er(1)-O(56)	2.35(3)
Er(1)-O(59)	2.45(3)	Er(1)-O(60)	2.18(3)		
O(41)-Er(1)-O(44)	77.3(10)	O(41)-Er(1)-O(47)	85.5(11)	O(41)-Er(1)-O(59)	73.2(10)
O(41)-Er(1)-O(50)	72.3(11)	O(41)-Er(1)-O(53)	143.6(9)	O(41)-Er(1)-O(56)	118.1(11)
O(44)-Er(1)-O(47)	77.6(10)	O(44)-Er(1)-O(50)	144.7(10)	O(44)-Er(1)-O(53)	122.2(9)
O(44)-Er(1)-O(56)	132.5(10)	O(44)-Er(1)-O(59)	72.3(9)	O(47)-Er(1)-O(50)	82.3(10)
O(47)-Er(1)-O(53)	71.4(9)	O(47)-Er(1)-O(59)	146.1(10)	O(50)-Er(1)-O(53)	76.9(9)
O(50)-Er(1)-O(59)	114.3(10)	O(53)-Er(1)-O(59)	139.1(8)	O(56)-Er(1)-O(47)	143.0(11)
O(56)-Er(1)-O(50)	79.0(10)	O(56)-Er(1)-O(53)	73.4(9)	O(56)-Er(1)-O(59)	70.9(10)
O(60)-Er(1)-O(41)	134.7(10)	O(60)-Er(1)-O(44)	65.1(10)	O(60)-Er(1)-O(47)	109.0(12)
O(60)-Er(1)-O(50)	150.0(10)	O(60)-Er(1)-O(53)	80.5(9)	O(60)-Er(1)-O(56)	75.7(11)
O(60)-Er(1)-O(59)	71.9(11)				

11					
Tm(1)-O(41)	2.300(6)	Tm(1)-O(44)	2.300(5)	Tm(1)-O(47)	2.290(5)
Tm(1)-O(50)	2.287(6)	Tm(1)-O(53)	2.272(6)	Tm(1)-O(56)	2.390(5)
Tm(1)-O(59)	2.359(5)	Tm(1)-O(60)	2.392(6)		
O(41)-Tm(1)-O(44)	77.75(19)	O(41)-Tm(1)-O(56)	122.9(2)	O(41)-Tm(1)-O(59)	69.20(19)
O(41)-Tm(1)-O(60)	71.6(2)	O(44)-Tm(1)-O(56)	141.22(16)	O(44)-Tm(1)-O(59)	142.74(19)
O(44)-Tm(1)-O(60)	73.58(18)	O(47)-Tm(1)-O(41)	146.60(18)	O(47)-Tm(1)-O(44)	74.22(18)
O(47)-Tm(1)-O(56)	73.08(17)	O(47)-Tm(1)-O(59)	142.31(19)	O(47)-Tm(1)-O(60)	116.2(2)
O(50)-Tm(1)-O(41)	75.1(2)	O(50)-Tm(1)-O(44)	78.9(2)	O(50)-Tm(1)-O(47)	82.0(2)
O(50)-Tm(1)-O(56)	76.5(2)	O(50)-Tm(1)-O(59)	107.7(2)	O(50)-Tm(1)-O(60)	140.3(2)
O(53)-Tm(1)-O(41)	133.15(18)	O(53)-Tm(1)-O(44)	114.8(2)	O(53)-Tm(1)-O(47)	76.25(18)
O(53)-Tm(1)-O(50)	149.3(2)	O(53)-Tm(1)-O(56)	76.6(2)	O(53)-Tm(1)-O(59)	78.6(2)
O(53)-Tm(1)-O(60)	69.9(2)	O(56)-Tm(1)-O(60)	140.89(18)	O(59)-Tm(1)-O(56)	74.08(18)
O(59)-Tm(1)-O(60)	79.9(2)				

Table S5 Weak interactions in the stacking structure of complex **1**.

Intermolecular hydrogen bonding within complex **1**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
C(2)-H(2A)···O(15)	0.97	2.43	3.30(2)
C(3)-H(3B)···O(14)	0.97	2.57	3.38(3)
C(11)-H(11A)···O(13)	0.97	2.39	3.21(2)
C(17)-H(17A)···O(5)	0.97	2.48	3.41(3)
C(18)-H(18B)···O(21)	0.96	2.35	3.27(2)
C(22)-H(22A)···O(37)	0.97	2.54	3.43(3)
C(23)-H(23B)···O(30)	0.97	2.46	3.31(3)
C(23)-H(23B)···O(44)	0.97	2.56	3.32(3)
C(31)-H(31A)···O(39)	0.97	2.58	3.47(3)
C(32)-H(32A)···O(44)	0.97	2.27	3.23(3)
C(35)-H(35A)···O(29)	0.97	2.57	3.26(3)
C(36)-H(36B)···O(34)	0.96	2.58	3.45(3)
C(42)-H(42A)···O(22)	0.96	2.57	3.49(3)
Intramolecular hydrogen bonding within complex **1**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
C(3)-H(3A)···O(54)	0.97	2.49	2.90(3)
C(13)-H(13A)···O(58)	0.97	2.58	3.00(2)

C(15)-H(15B)···O(47)	0.97	2.44	2.78(3)
C(25)-H(25A)···O(49)	0.97	2.36	2.88(3)
C(33)-H(33A)···O(66)	0.97	2.54	2.97(3)
C(37)-H(37A)···O(52)	0.96	2.39	2.84(3)

Table S6 Weak interactions in the stacking structure of complex **2**.

Intermolecular hydrogen bonding within complex **2**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.87	2.23	2.9497
C(4)-H(4A)···O(24)	0.96	2.59	3.5406
C(24)-H(24B)···O(30)	0.96	1.95	2.9016
C(27)-H(27A)···O(40)	0.96	2.52	3.4248
C(35)-H(35B)···O(35)	0.96	1.79	2.4083

Intramolecular hydrogen bonding within complex **2**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59B)···O(47)	0.87	2.50	2.9748
C(5)-H(5B)···O(41)	0.96	2.59	3.1837
C(7)-H(7C)···O(42)	0.96	2.59	3.2624
C(17)-H(17)···O(49)	0.98	2.51	2.9265
C(24)-H(24C)···O(50)	0.96	1.89	2.8014
C(24)-H(24C)···O(59)	0.96	2.54	3.0421
C(33)-H(33B)···O(55)	0.96	2.56	3.3431
C(35)-H(35C)···O(54)	0.96	2.14	2.6917

Table S7 Weak interactions in the stacking structure of complex **3**.

Intermolecular hydrogen bonding within complex **3**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.85	2.13	2.8471
C(1)-H(1A)···O(33)	0.97	2.52	3.4144
C(4)-H(4A)···O(24)	0.96	2.56	3.4429
C(10)-H(10C)···O(34)	0.96	2.60	3.4759
C(15)-H(15B)···O(10)	0.97	2.57	3.3034
C(16)-H(16B)···O(10)	0.97	2.52	3.2459
C(21)-H(21A)···O(39)	0.96	2.53	3.4810
C(24)-H(24C)···O(30)	0.96	1.93	2.8097

C(27)-H(27A)···O(40)	0.96	2.59	3.4540
C(35)-H(35B)···O(35)	0.96	1.64	2.2441

Intramolecular hydrogen bonding within complex **3**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59B)···O(47)	0.85	2.51	2.9586
C(5)-H(5B)···O(41)	0.96	2.52	3.2188
C(7)-H(7C)···O(42)	0.96	2.59	3.2432
C(16)-H(16A)···O(49)	0.97	2.53	3.0790
C(17)-H(17)···O(49)	0.98	2.56	2.9689
C(20)-H(20)···O(47)	0.98	2.55	3.0328
C(24)-H(24A)···O(50)	0.96	2.11	2.9689
C(24)-H(24A)···O(59)	0.96	2.38	3.0663
C(35)-H(35A)···O(54)	0.96	1.80	2.7127

Table S8 Weak interactions in the stacking structure of complex **4**.

Intermolecular hydrogen bonding within complex **4**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.86	2.20	2.92(4)
C(1)-H(1A)···O(33)	0.97	2.52	3.44(3)
C(4)-H(4B)···O(24)	0.96	2.58	3.53(3)
C(16)-H(16B)···O(10)	0.97	2.47	3.21(3)
C(21)-H(21A)···O(39)	0.96	2.56	3.50(3)
C(24)-H(24B)···O(30)	0.96	2.15	3.10(4)
C(27)-H(27A)···O(40)	0.96	2.56	3.46(3)
C(35)-H(35B)···O(35)	0.96	1.70	2.43(4)
C(39)-H(39C)···O(31)	0.96	2.58	3.40(4)

Intramolecular hydrogen bonding within complex **4**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59B)···O(47)	0.86	2.44	2.88(4)
C(7)-H(7C)···O(42)	0.96	2.53	3.18(3)
C(13)-H(13B)···O(53)	0.96	2.27	3.22(3)
C(13)-H(13B)···O(53)	0.96	2.57	2.98(3)
C(13)-H(13C)···O(53)	0.96	2.23	2.98(3)
C(16)-H(16A)···O(49)	0.97	2.53	3.07(4)
C(24)-H(24C)···O(50)	0.96	2.10	2.95(4)

C(30)-H(30A)···O(55)	0.97	2.48	2.99(3)
C(35)-H(35C)···O(54)	0.96	1.99	2.88(3)

Table S9 Weak interactions in the stacking structure of complex **5**.

Intermolecular hydrogen bonding within complex **5**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(63)-H(63B)···N(2)	0.85	2.13	2.8608
O(64)-H(64B)···N(1)	0.85	2.03	2.8109
O(64)-H(64C)···O(6)	0.85	2.21	2.8982
C(5)-H(5B)···O(12)	0.98	2.46	3.3456
C(6)-H(6A)···O(14)	0.99	2.55	3.2802
C(11)-H(11C)···O(9)	0.98	2.60	3.5420
C(11)-H(11C)···O(17)	0.98	2.58	3.2986
C(13)-H(13A)···O(14)	0.99	2.52	3.2954
C(19)-H(19A)···O(4)	0.98	2.54	3.5104
C(19)-H(19B)···O(4)	0.98	2.48	3.4450
C(22)-H(22B)···O(3)	0.98	2.48	3.4147
C(24)-H(24C)···O(24)	0.98	2.46	3.3540
C(30)-H(30A)···O(16)	0.99	2.59	3.3529
C(39)-H(39A)···N(4)	0.98	2.47	3.3854
C(46)-H(46C)···O(24)	0.98	2.57	3.3972
C(51)-H(51A)···O(1)	0.98	2.56	3.4019

Intramolecular hydrogen bonding within complex **5**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(64)-H(64C)···O(63)	0.85	2.56	2.8986
C(6)-H(6B)···O(61)	0.99	2.55	3.0826
C(7)-H(7B)···O(61)	1.00	2.54	2.9674
C(10)-H(10B)···O(60)	1.00	2.52	3.0233
C(17)-H(17A)···O(48)	0.98	2.51	3.2309

Table S10 Weak interactions in the stacking structure of complex **6**.

Intermolecular hydrogen bonding within complex **6**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.87	2.26	2.9931
C(21)-H(21B)···O(39)	0.96	2.59	3.5270

C(24)-H(24A)···O(30)	0.96	2.31	3.1806
C(27)-H(27A)···O(40)	0.96	2.51	3.4004
C(35)-H(35B)···O(11)	0.96	2.53	3.3761
C(35)-H(35B)···O(35)	0.96	1.66	2.2651
Intramolecular hydrogen bonding within complex **6**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59B)···O(47)	0.86	2.42	2.8680
O(60)-H(60A)···O(53)	0.87	2.60	2.9336
C(20)-H(20)···O(47)	0.98	2.53	3.0231
C(24)-H(24B)···O(50)	0.96	2.37	3.1711
C(33)-H(33B)···O(55)	0.96	2.24	3.0851
C(35)-H(35C)···O(54)	0.96	2.25	2.9220

Table S11 Weak interactions in the stacking structure of complex **7**.

Intermolecular hydrogen bonding within complex **7**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.86	2.28	2.9825
C(1)-H(1A)···O(33)	0.97	2.50	3.3781
C(4)-H(4A)···O(24)	0.96	2.51	3.4293
C(10)-H(10A)···O(34)	0.96	2.54	3.4298
C(13)-H(13A)···O(36)	0.96	2.58	3.5374
C(21)-H(21A)···O(23)	0.96	2.59	3.3043
C(24)-H(24C)···O(30)	0.96	1.90	2.6978
C(27)-H(27A)···O(40)	0.96	2.52	3.3981
C(35)-H(35B)···O(35)	0.96	1.84	2.2683
Intramolecular hydrogen bonding within complex **7**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(60)	0.86	2.55	2.8319
O(59)-H(59B)···O(47)	0.86	2.37	2.8267
O(60)-H(60A)···O(53)	0.86	2.56	2.8767
C(16)-H(16A)···O(49)	0.97	2.53	3.1130
C(17)-H(17)···O(49)	0.98	2.52	2.9404
C(20)-H(20)···O(47)	0.98	2.55	3.0621
C(24)-H(33C)···O(50)	0.96	2.46	3.0854
C(33)-H(35C)···O(55)	0.96	2.30	3.0911

C(35)-H(35C)···O(54)	0.96	2.02	2.9053

Table S12 Weak interactions in the stacking structure of complex **8**.

Intermolecular hydrogen bonding within complex **8**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.86	2.19	2.9051
C(1)-H(1A)···O(33)	0.97	2.49	3.3916
C(4)-H(4B)···O(24)	0.96	2.55	3.4904
C(6)-H(6)···O(15)	0.98	2.58	3.5322
C(13)-H(13B)···O(17)	0.96	2.46	3.3977
C(24)-H(24A)···O(30)	0.96	2.33	3.2849
C(25)-H(25A)···O(5)	0.96	2.59	3.5322
C(27)-H(27A)···O(40)	0.96	2.60	3.5004
C(30)-H(30B)···O(7)	0.97	2.50	3.3158
C(35)-H(35A)···O(35)	0.96	1.78	2.3053
C(35)-H(35B)···O(17)	0.96	2.55	3.4327

Intramolecular hydrogen bonding within complex **8**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(60)-H(60A)···O(53)	0.87	2.59	2.8791
C(17)-H(17)···O(49)	0.98	2.56	2.9494
C(24)-H(24A)···O(59)	0.96	2.54	2.9861
C(24)-H(24B)···O(50)	0.96	1.73	2.6275
C(33)-H(33A)···O(55)	0.96	2.45	3.1656
C(35)-H(35C)···O(54)	0.96	2.06	2.9783

Table S13 Weak interactions in the stacking structure of complex **9**.

Intermolecular hydrogen bonding within complex **9**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···N(1)	0.88	2.27	3.0788
O(60)-H(60A)···O(6)	0.87	2.26	2.9110
O(60)-H(60B)···N(3)	0.87	2.02	2.8196
C(6)-H(6B)···O(17)	0.96	2.49	3.3442
C(7)-H(7B)···O(27)	0.97	2.57	3.2704
C(8)-H(8B)···O(27)	0.97	2.54	3.2936
C(11)-H(11B)···O(35)	0.96	2.59	3.2710

C(17)-H(17B)···O(25)	0.96	2.56	3.5045
C(17)-H(17C)···O(25)	0.96	2.54	3.4819
C(22)-H(22A)···O(16)	0.97	2.50	3.4057
C(28)-H(28B)···O(18)	0.96	2.52	3.3503
C(29)-H(29B)···O(19)	0.96	2.55	3.3696
C(32)-H(32C)···O(12)	0.96	2.56	3.4222
C(40)-H(40B)···N(4)	0.96	2.54	3.4108
C(45)-H(45B)···O(18)	0.96	2.59	3.4057
Intramolecular hydrogen bonding within complex **9**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59B)···O(60)	0.88	2.51	2.8570
O(60)-H(60A)···O(59)	0.87	2.49	2.8570
C(7)-H(7A)···O(45)	0.97	2.53	3.0556
C(13)-H(13)···O(45)	0.98	2.54	2.9397
C(20)-H(20A)···O(47)	0.96	2.55	3.2716
C(25)-H(25C)···O(52)	0.96	2.60	3.2511

Table S14 Weak interactions in the stacking structure of complex **10**.

Intermolecular hydrogen bonding within complex **10**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(30)	0.85	2.09	2.9066
O(60)-H(60D)···O(21)	0.85	2.11	2.9556
O(1)-H(1B)···O(37)	0.97	2.41	3.3776
C(3)-H(3)···O(37)	0.98	2.41	3.3018
C(10)-H(10A)···O(9)	0.96	2.59	3.5432
C(16)-H(16B)···O(40)	0.97	2.56	3.5271
C(27)-H(27C)···O(22)	0.96	2.29	3.1795
C(38)-H(38A)···O(27)	0.96	2.37	3.2720
C(39)-H(39B)···O(30)	0.96	2.11	2.6685
C(39)-H(39C)···O(23)	0.96	1.86	2.5089
C(41)-H(41A)···O(9)	0.96	2.54	3.4058
Intramolecular hydrogen bonding within complex **10**			
Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(60)-H(60C)···O(53)	0.85	2.48	2.9930
O(60)-H(60C)···O(54)	0.85	2.21	3.0591

C(6)-H(6)···O(41)	0.98	2.44	2.9722
C(15)-H(15B)···O(15)	0.97	2.38	3.2159
C(20)-H(20)···O(12)	0.98	2.20	2.8927
C(22)-H(22A)···O(14)	0.96	2.33	3.1966
C(22)-H(22B)···O(15)	0.96	1.97	2.5721
C(30)-H(30A)···O(52)	0.96	2.60	3.5579
C(39)-H(39B)···O(58)	0.96	2.29	3.0666

Table S15 Weak interactions in the stacking structure of complex **11**.

Intermolecular hydrogen bonding within complex **11**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(60)-H(60A)···N(2)	0.88	2.03	2.8781
O(60)-H(60B)···O(40)	0.88	2.11	2.9243
C(3)-H(3B)···O(64)	0.98	2.39	3.3122
C(6)-H(6B)···O(2)	0.98	2.54	3.4049
C(7)-H(7B)···O(9)	0.99	2.57	3.3607
C(18)-H(18A)···O(9)	0.98	2.55	3.5039
C(18)-H(18C)···O(62)	0.98	2.42	3.2109
C(19)-H(19)···O(31)	1.00	2.50	3.4030
C(21)-H(21B)···O(32)	0.99	2.53	3.3062
C(22)-H(22A)···O(19)	0.99	2.31	3.1732
C(22)-H(22B)···O(20)	0.99	2.40	3.1919
C(26)-H(22B)···O(15)	0.98	2.31	3.2828
C(30)-H(30)···O(37)	1.00	2.36	3.3103
C(35)-H(35B)···O(37)	0.99	2.51	3.5028
C(40)-H(40B)···O(63)	0.98	2.55	3.2972
C(46)-H(46B)···O(22)	0.98	2.20	3.0568
C(46)-H(46C)···O(35)	0.98	2.56	3.2871

Intramolecular hydrogen bonding within complex **11**

Donor-H···Acceptor	D-H (Å)	H-A (Å)	D-A (Å)
O(59)-H(59A)···O(57)	0.89	2.40	2.8013
O(59)-H(59B)···O(57)	0.89	2.40	2.8013
O(60)-H(60B)···O(53)	0.88	2.37	2.6742
C(7)-H(7A)···O(48)	0.99	2.58	3.5692
C(10)-H(10)···O(51)	1.00	2.58	3.5438

C(19)-H(19)···O(49)	1.00	2.42	2.8589
C(33)-H(33)···O(44)	1.00	2.52	2.9748
C(41)-H(41)···O(43)	1.00	2.59	3.0328