Supporting Information

The supporting information contains 9 pages，including 11 tables and 2 figure.

Table S1. Summary of the thermodynamic constants from the databases

Parameter	Value	Reference
pK_{a1} (H_2Ox)	1.19	ThermoChimie
pK_{a2} (HOx^-)	3.83	ThermoChimie
$\log \beta_{1,1}$ ($Eu(OH)^{2+}$)	-7.64	PSINA
$\log \beta_{1,2}$ ($Eu(OH)_2^+$)	-15.1	PSINA
$\log \beta_{1,3}$ ($Eu(OH)_3$)	-23.7	PSINA
$\log k_1$ ($Eu(Ox)^+$)	6.55	ThermoChimie
$\log k_2$ ($Eu(Ox)_2^-$)	10.93	ThermoChimie
$\log k_3$ ($Eu(Ox)_3^{3-}$)	12.48	ThermoChimie

Table S2. Fractional weights of various species of Eu(III)(10 μM) or Ox(10 mM) under different pH obtained from theoretical calculation in 0.1 M $NaClO_4$, 25 ℃

pH	$Eu^{3+}{}_{(aq)}$	$Eu(OH)^{2+}$	$Eu(OH)_2^+$	$Eu(OH)_3$	HOx^-	Ox^{2-}
3.0	100	*	\	\	87.5	10.8
3.2	100	\	\	\	82.7	16.3
3.4	100	\	\	\	75.7	23.7
3.6	100	\	\	\	66.5	33.2
3.8	100	\	\	\	55.7	44.2
4.0	100	\	\	\	44.1	55.8
4.2	100	\	\	\	33.2	66.8
4.4	100	\	\	\	23.8	76.2
4.6	100	\	\	\	16.4	83.6
4.8	100	\	\	\	11.0	89.0
5.0	99.9	\	\	\	7.2	92.8
5.2	99.9	0.1	\	\	4.7	95.3
5.4	99.8	0.2	\	\	3.0	97.0
5.6	99.7	0.3	\	\	1.9	98.1
5.8	99.6	0.4	\	\	1.2	98.8
6.0	99.3	0.7	\	\	0.8	99.2
6.2	98.9	1.0	\	\	0.5	99.5

6.4	98.3	1.6	\	\	0.3	99.7
6.6	97.3	2.6	0.2	\	0.2	99.8
6.8	95.6	4.0	0.4	\	0.1	99.9
7.0	92.9	6.1	1.0	\	\	99.9
7.2	88.3	9.2	2.4	\	\	100
7.4	80.8	13.4	5.5	0.3	\	100
7.6	69.1	18.1	11.9	0.9	\	100
7.8	52.6	21.9	22.7	2.8	\	100
8.0	33.9	22.3	36.7	7.2	\	100
8.2	17.8	18.7	48.5	15.0	\	100
8.4	7.8	12.9	53.2	26.1	\	100
8.6	2.9	7.7	50.3	39.1	\	100
8.8	1.0	4.1	42.5	52.4	\	100
9.0	0.3	2.0	33.1	64.6	\	100
9.2	\	0.9	24.2	74.8	\	100
9.4	\	0.4	16.9	82.6	\	100

*Less than 0.1%

Table S3. Fractional weights(%) of various species of Eu(III)–Ox complexes obtained from theoretical calculation for the 10 μM Eu(III) and various concentration of Ox in 0.1 M $NaClO_4$ at pH 5.5, 25 ℃

[Ox]/mM	Eu^{3+}	$Eu(Ox)^{+}$	$Eu(Ox)_2^{-}$	$Eu(Ox)_3^{3-}$
0	100	*	\	\
0.005	72.7	26.7	0.5	\
0.01	53.1	44.9	1.9	\
0.02	30.6	62.7	6.6	\
0.05	10.5	67.3	22.1	\
0.1	3.9	55.4	40.3	0.3
0.2	1.3	38.3	59.4	1.0
0.5	0.2	19.1	77.2	3.5
1	\	10.0	82.2	7.7
2	\	4.9	79.9	15.2
5	\	1.6	65.9	32.5
10	\	0.6	48.9	50.4
20	\	0.2	31.0	68.8
30	\	0.1	22.0	77.9
50	\	\	13.3	86.7

*Less than 0.1%

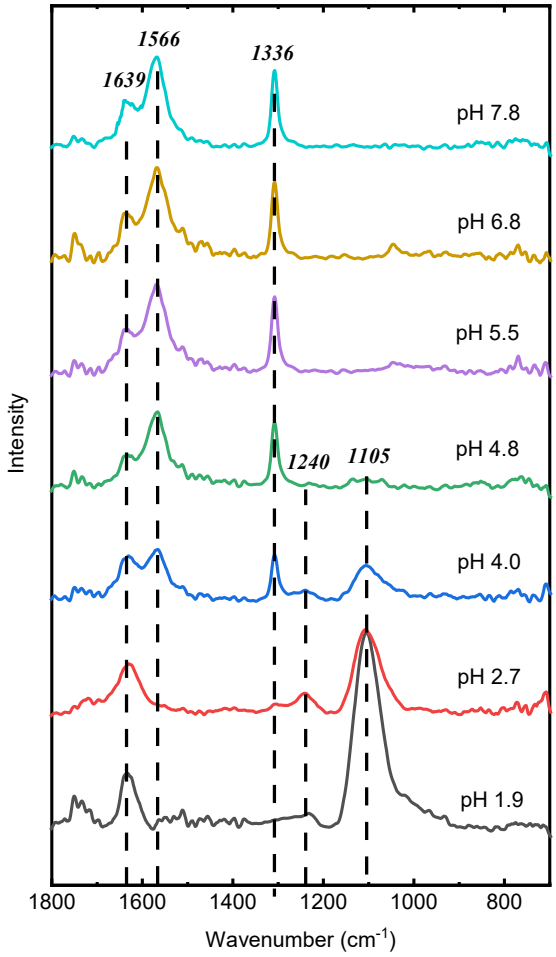

Fig. S1 ATR-FTIR spectral of aqueous Ox (10 mM) at different solution pH values. All ATR-FTIR spectra were recorded for 2048 scans in the range of 600 to 2000 cm^{-1} per sample with the spectrum spotlight 200 FT-IR microscopy (PerkinElmer, U.S.) equipping with the ATR accessory in air atmosphere at room temperature (298 ± 2 K).

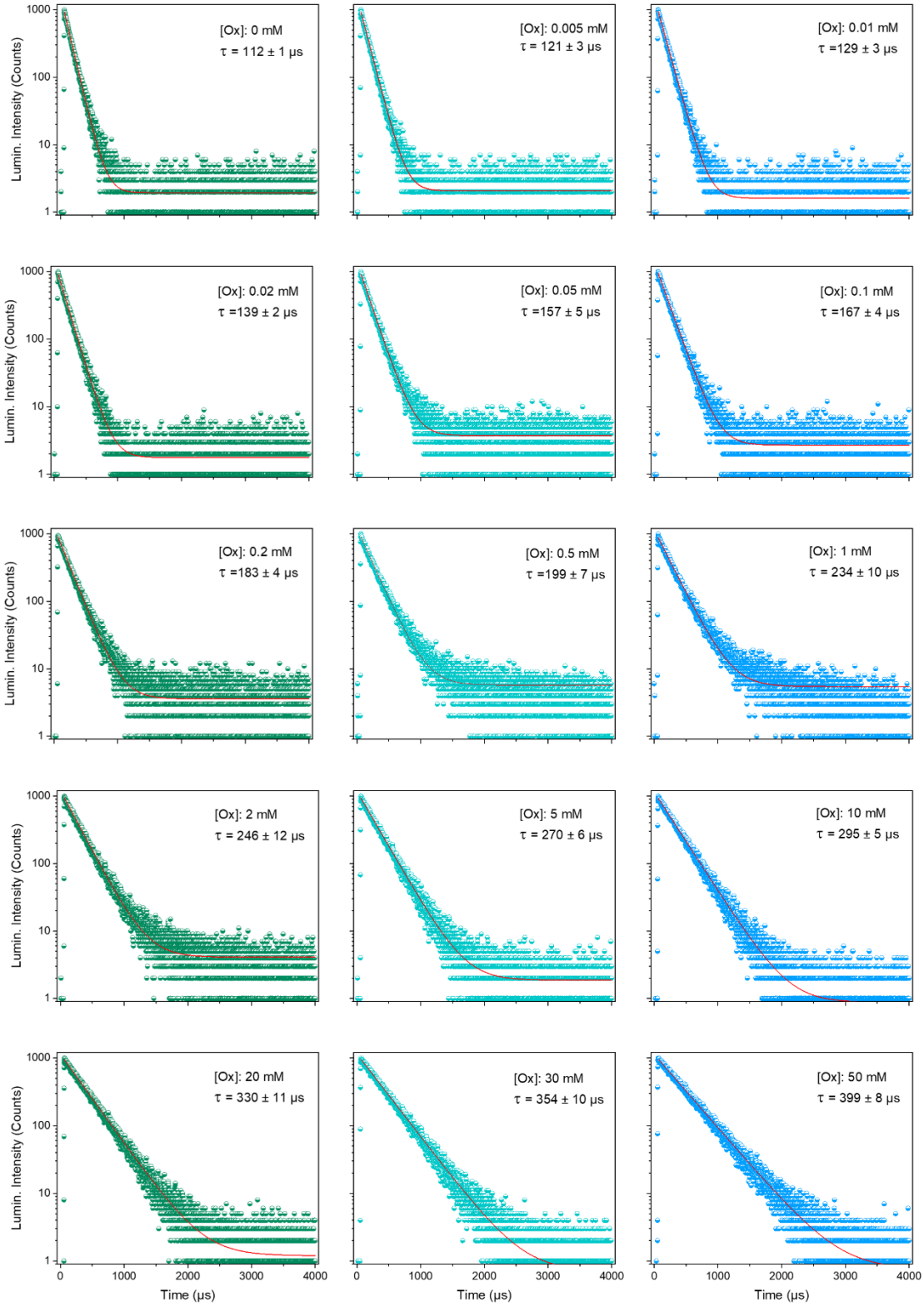

Fig. S2 Representative luminescence decay curves of the samples comprising 10 μM Eu(III) and various concentration of Ox in 0.1 M $NaClO_4$ at pH 5.5. The red lines are the ftting lines; λ_{ex} = 394 nm, λ_{em} = 616 nm.

Table S4a. Detailed structural and electronic information of $Eu(H_2O)_9^{3+}$

Atom	X	Y	Z	Mulliken charge
Eu	-0.003730	-0.049213	-0.016315	1.944
O	-1.924820	-1.720940	0.034408	-0.656
H	-2.756816	-1.260482	-0.127878	0.391
O	1.753365	0.929697	1.566635	-0.657
H	1.943618	0.270452	2.245190	0.388
O	-1.769756	1.012114	1.515041	-0.659
H	-1.708313	1.925027	1.205898	0.389
O	-0.055371	2.686977	-0.026639	-0.692
H	-0.145773	2.926142	-0.955595	0.393
O	1.883418	0.888077	-1.474332	-0.659
H	2.049763	1.813021	-1.261766	0.385
O	-1.807684	0.907898	-1.542223	-0.656
H	-1.919623	0.214960	-2.205021	0.392
O	-0.076970	-1.316003	-2.235545	-0.672
H	0.789979	-1.341766	-2.654997	0.395
O	1.905677	-1.745892	0.039732	-0.659
H	2.645854	-1.334934	0.500874	0.389
O	-0.139130	-1.354955	2.201703	-0.672
H	0.698906	-1.780416	2.406466	0.394
H	-1.929018	-1.942949	0.974815	0.391
H	2.582298	1.037752	1.086197	0.388
H	-2.659145	0.717003	1.287291	0.391
H	0.803129	3.025571	0.245858	0.388
H	2.706354	0.431167	-1.262941	0.388
H	-2.647378	0.953978	-1.072576	0.390
H	-0.306031	-2.23659	-2.060255	0.397
H	2.221357	-1.898895	-0.859193	0.392
H	-0.284026	-0.714428	2.905248	0.397

Table S4b. Detailed bond length and bond order information of $Eu(H_2O)_9^{3+}$

Central atom	Coordination atom	Bond length	Mayer bond order
Eu	O2	2.547	0.240
Eu	O4	2.560	0.222
Eu	O6	2.567	0.230
Eu	O8	2.737	0.139
Eu	O10	2.562	0.216

Eu	O12	2.549	0.234
Eu	O14	2.556	0.206
Eu	O16	2.555	0.225
Eu	O18	2.577	0.202

Table S5a. Detailed structural and electronic information of $Eu(Ox)_1(H_2O)_7^+$

Atom	X	Y	Z	Mulliken charge
Eu	0.547334	0.012203	0.000373	1.777
O	1.631919	1.826933	1.433156	-0.664
H	2.535891	1.534722	1.616065	0.395
O	-0.094590	-0.184420	2.525187	-0.667
H	-1.050730	-0.329380	2.539377	0.392
O	2.252048	-1.160830	1.557941	-0.663
H	2.109299	-2.044070	1.182935	0.388
O	2.741292	-0.041730	-1.335610	-0.672
H	2.410095	-0.323970	-2.200930	0.393
O	0.762104	2.349552	-1.186700	-0.676
H	-0.190220	2.523152	-1.105070	0.383
O	0.842060	-2.478300	-0.616420	-0.666
H	0.986290	-2.540130	-1.570810	0.391
O	-0.074400	-0.282770	-2.478950	-0.668
H	-0.742600	-0.982660	-2.505470	0.391
H	-0.555310	0.511526	-2.751300	0.389
H	0.915524	2.251477	-2.136390	0.395
H	1.728894	2.485064	0.726605	0.390
H	0.019989	0.740969	2.787580	0.394
H	3.247327	-0.804070	-1.020970	0.394
H	-0.118060	-2.604270	-0.504650	0.379
H	1.632074	-1.121430	2.306306	0.387
C	-2.577160	-0.785060	0.070955	0.293
O	-1.418130	-1.314770	0.165211	-0.552
O	-3.644620	-1.385150	-0.028330	-0.524
C	-2.575270	0.771127	0.085355	0.283
O	-3.64600	1.372681	0.043740	-0.525
O	-1.413680	1.301047	0.130192	-0.535

Table S5b. Detailed bond length and bond order information of $Eu(Ox)_1(H_2O)_7^+$

Central atom	Coordination atom	Bond length	Mayer bond order
Eu	O2	2.554	0.227
Eu	O4	2.613	0.200
Eu	O6	2.590	0.239
Eu	O8	2.569	0.209
Eu	O10	2.630	0.193
Eu	O12	2.583	0.220
Eu	O14	2.573	0.205
Eu	O24	2.377	0.328
Eu	O28	2.350	0.346

Table S6a. Detailed structural and electronic information of $Eu(Ox)_2(H_2O)_4^-$

Atom	X	Y	Z	Mulliken charge
Eu	0.031584	-0.467700	-0.089890	1.805
O	0.382352	-0.774980	2.456897	-0.672
H	-0.309850	-0.104620	2.600500	0.380
O	-1.198340	-2.594060	0.713645	-0.669
H	-2.106420	-2.330900	0.503181	0.387
O	0.790681	-2.562860	-1.432510	-0.683
H	1.678251	-2.416130	-1.058350	0.378
O	0.035397	0.482468	-2.426740	-0.687
H	-0.087420	1.429325	-2.151820	0.374
O	-0.256410	2.890627	-1.279350	-0.724
H	-1.108930	2.770555	-0.837610	0.381
H	0.389849	2.565380	-0.610230	0.366
H	1.204387	-0.324880	2.696017	0.389
H	-1.141630	-2.514020	1.676670	0.389
H	-0.864080	0.202279	-2.655400	0.379
H	0.382045	-3.209480	-0.838100	0.387
C	-3.118970	0.239571	-0.401450	0.292
O	-2.200680	-0.438120	-0.968570	-0.556
O	-4.265180	0.405325	-0.820880	-0.539
C	-2.710610	0.897179	0.951472	0.284
O	-3.565660	1.478757	1.617719	-0.532
O	-1.478500	0.766661	1.261939	-0.555
C	3.250774	-0.042400	0.159778	0.296
O	2.378882	-0.957130	-0.013360	-0.554

O	4.469879	-0.198580	0.208042	-0.533
C	2.670775	1.395767	0.308605	0.316
O	3.442784	2.344425	0.419594	-0.529
O	1.392556	1.464598	0.292062	-0.572

Table S6b. Detailed bond length and bond order information of $Eu(Ox)_2(H_2O)_4^-$

Central atom	Coordination atom	Bond length	Mayer bond order
Eu	O2	2.589	0.219
Eu	O4	2.585	0.203
Eu	O6	2.602	0.207
Eu	O8	2.523	0.250
Eu	O18	2.399	0.304
Eu	O22	2.373	0.309
Eu	O24	2.399	0.298
Eu	O28	2.394	0.297

Table S7a. Detailed structural and electronic information of $Eu(Ox)_3(H_2O)_2^{3-}$

Atom	X	Y	Z	Mulliken charge
Eu	-0.043720	-0.093390	-0.401370	1.810
C	1.473718	2.349583	1.084027	0.271
O	1.134836	1.135481	1.253756	-0.526
O	2.018896	3.076350	1.918851	-0.549
C	1.152235	2.943493	-0.320850	0.299
O	1.423375	4.122653	-0.549520	-0.541
O	0.613048	2.125858	-1.138960	-0.582
C	-3.175740	-0.952430	0.116517	0.283
O	-2.088880	-1.442190	-0.333250	-0.573
O	-4.288380	-1.477870	0.052973	-0.540
C	-3.042400	0.447239	0.790789	0.294
O	-4.067610	1.028580	1.149868	-0.535
O	-1.849530	0.883562	0.918551	-0.572
C	2.889015	-1.463240	-0.394820	0.290
O	2.187686	-0.633960	-1.055380	-0.547
O	4.075491	-1.737590	-0.594110	-0.552
C	2.145120	-2.177380	0.773414	0.304
O	2.768960	-2.948680	1.502184	-0.541

O	0.905573	-1.887290	0.873865	-0.578
O	-1.540380	1.090219	-2.234370	-0.684
H	-1.345920	0.678279	-3.086910	0.380
O	-0.391030	-1.943490	-2.247060	-0.690
H	-1.268320	-2.034960	-1.823010	0.370
O	-0.948430	-1.146510	2.807931	-0.755
H	-1.214680	-0.356570	2.309636	0.356
H	-0.247640	-1.521000	2.240909	0.357
H	-0.578300	-1.525450	-3.097700	0.383
H	-0.871360	1.798661	-2.153730	0.372

Table S7b. Detailed bond length and bond order information of $Eu(Ox)_3(H_2O)_2^{3-}$

Central atom	Coordination atom	Bond length	Mayer bond order
Eu	O3	2.375	0.315
Eu	O7	2.429	0.261
Eu	O9	2.451	0.257
Eu	O13	2.441	0.250
Eu	O15	2.387	0.302
Eu	O19	2.397	0.274
Eu	O20	2.646	0.188
Eu	O22	2.636	0.178