The Role of Ligand to Metal Charge-Transfer States on the Luminescence of Europium complexes with 18-Memberred Macrocyclic Ligands

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Electronic Supplementary Information(ESI)

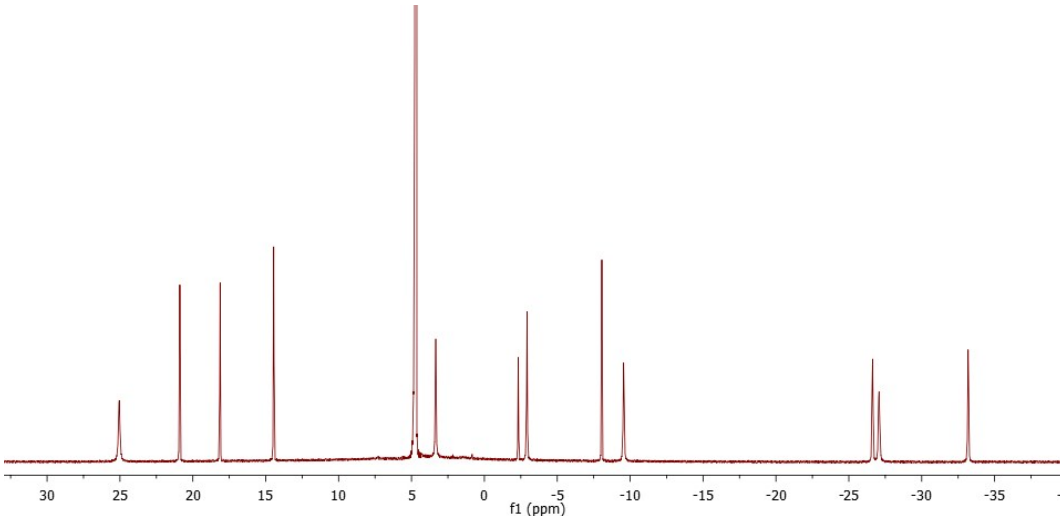


Figure S1. The ^{1}H NMR spectrum of $[EuL^{1}](NO_3)_3 \cdot 4H_2O$ recorded in D_2O solution at neutral pH and 25 ºC.

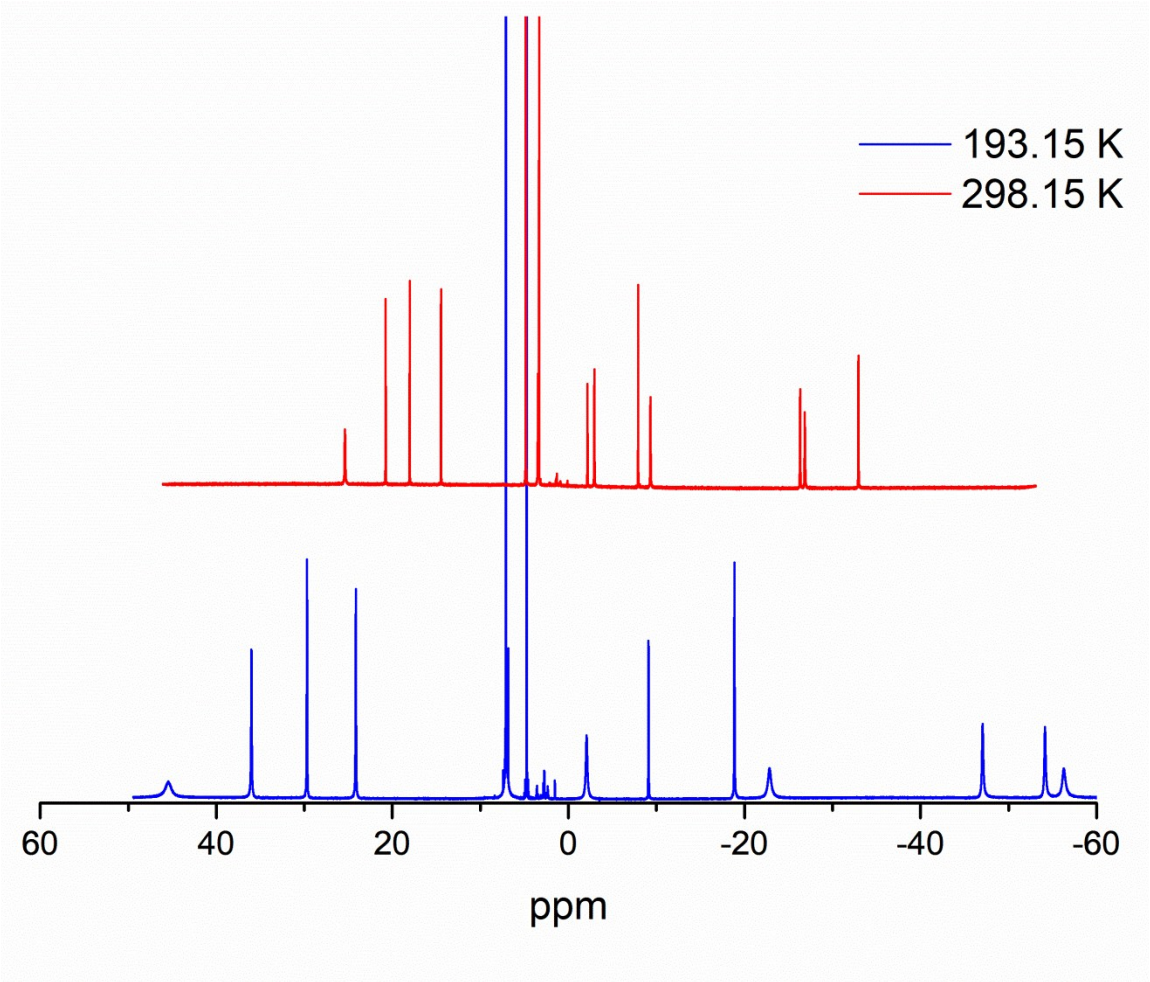


Figure S2. The ^{1}H NMR spectrum of [EuL^{1}](NO$_3$)$_3$·4H$_2$O recorded in d_3-MeOD solution at different temperatures.

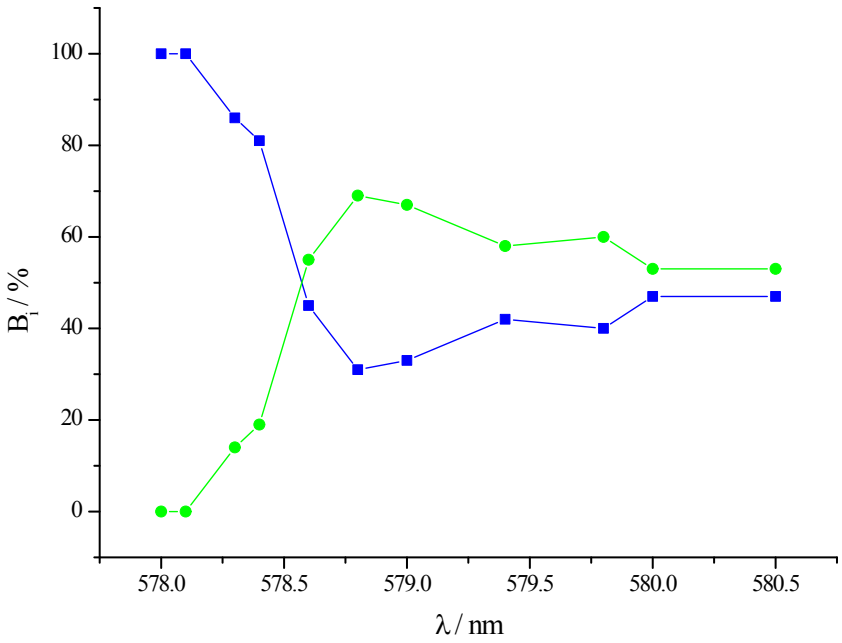


Figure S3. Variations of the pre-exponential factors (B_i) of the species obtained from the fitting of the emission decays of $[EuL^1]^{3+}$ (see text for full details) at various emission wavelengths by fixing $\tau_1 = 2.11$ ms (▪) and varying τ_2 (●).

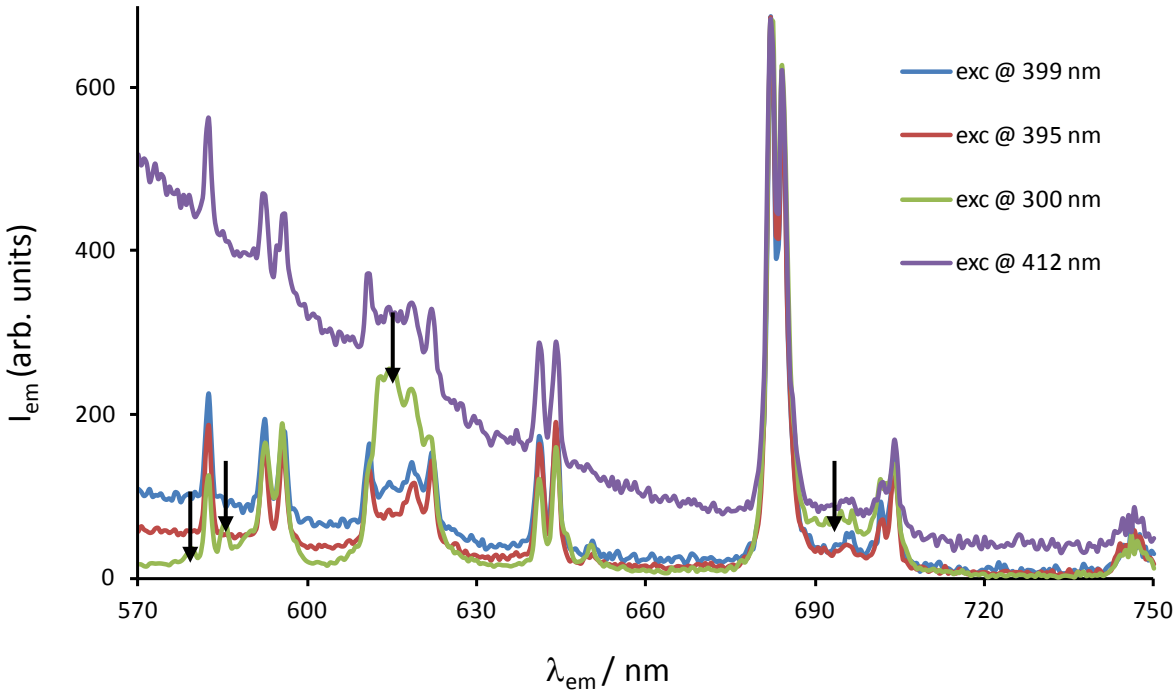


Figure S4. Emission spectra of $[EuL^1]^{3+}$ (H_2O, 4.92×10^{-3} M, pH 7.0) recorded upon excitation at 300, 395, 399 and 412 nm (exc slits = 1.0 nm, emission slits = 1.0 nm, filter at 395 nm). The appearance of some apparent broad emission at high energy when increasing the excitation wavelength may be related to the emission of the Raman band of water

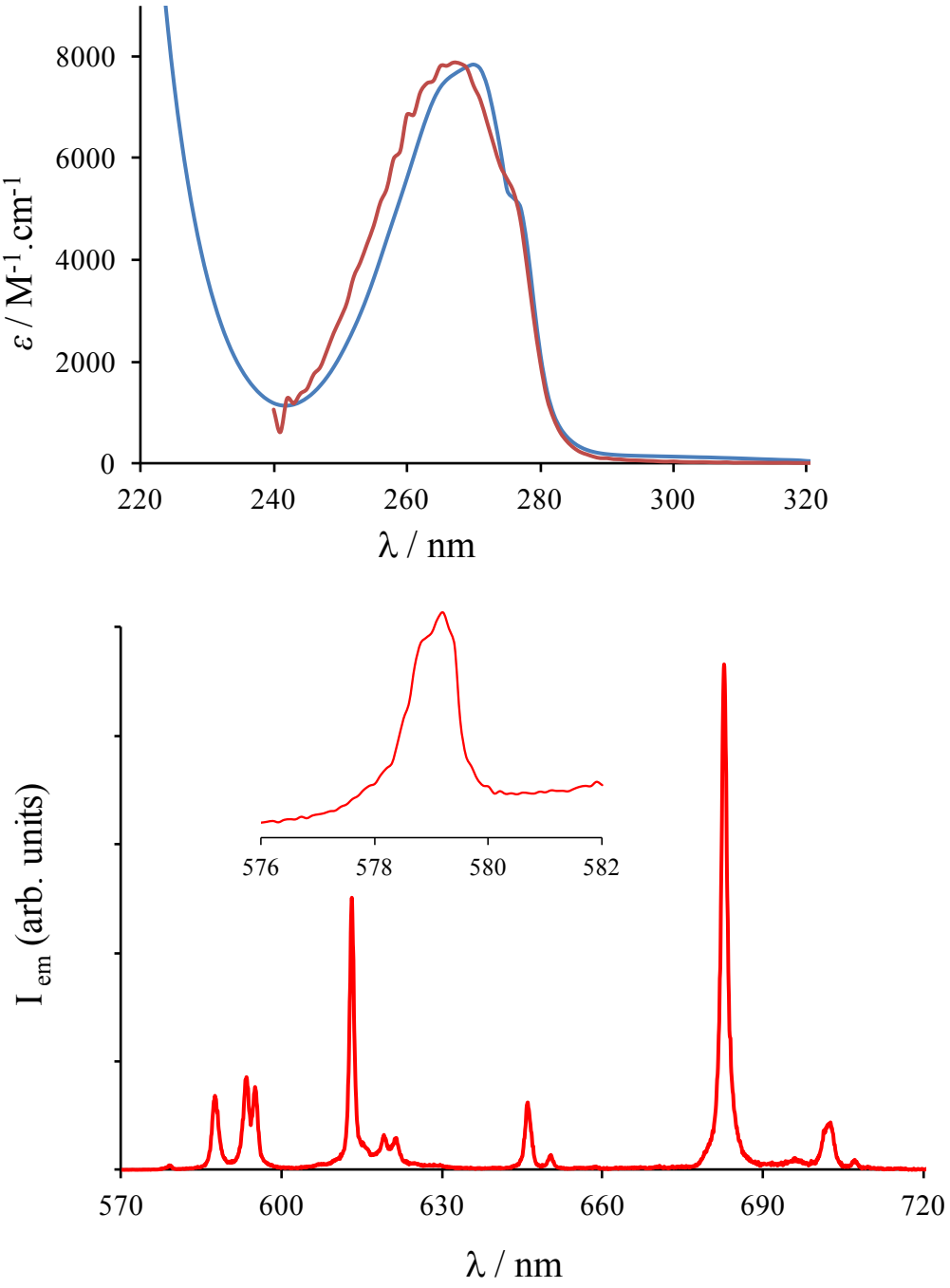


Figure S5. UV/Vis absorption spectra (blue: pH = 7.0, 1.27×10^{-4} M), excitation spectra (red: pH = 7.0, 3.8×10^{-4} M, λ_{em} = 592 nm) and high resolution emission spectra (red: pH = 7.0, 3.81×10^{-4} M, λ_{exc} = 279 nm) recorded in aqueous solution at r.t for the $[EuL^2](NO_3)_3$ complex with enlargement of the $^5D_0 \rightarrow {}^7F_0$ transition at 1 Å resolution.

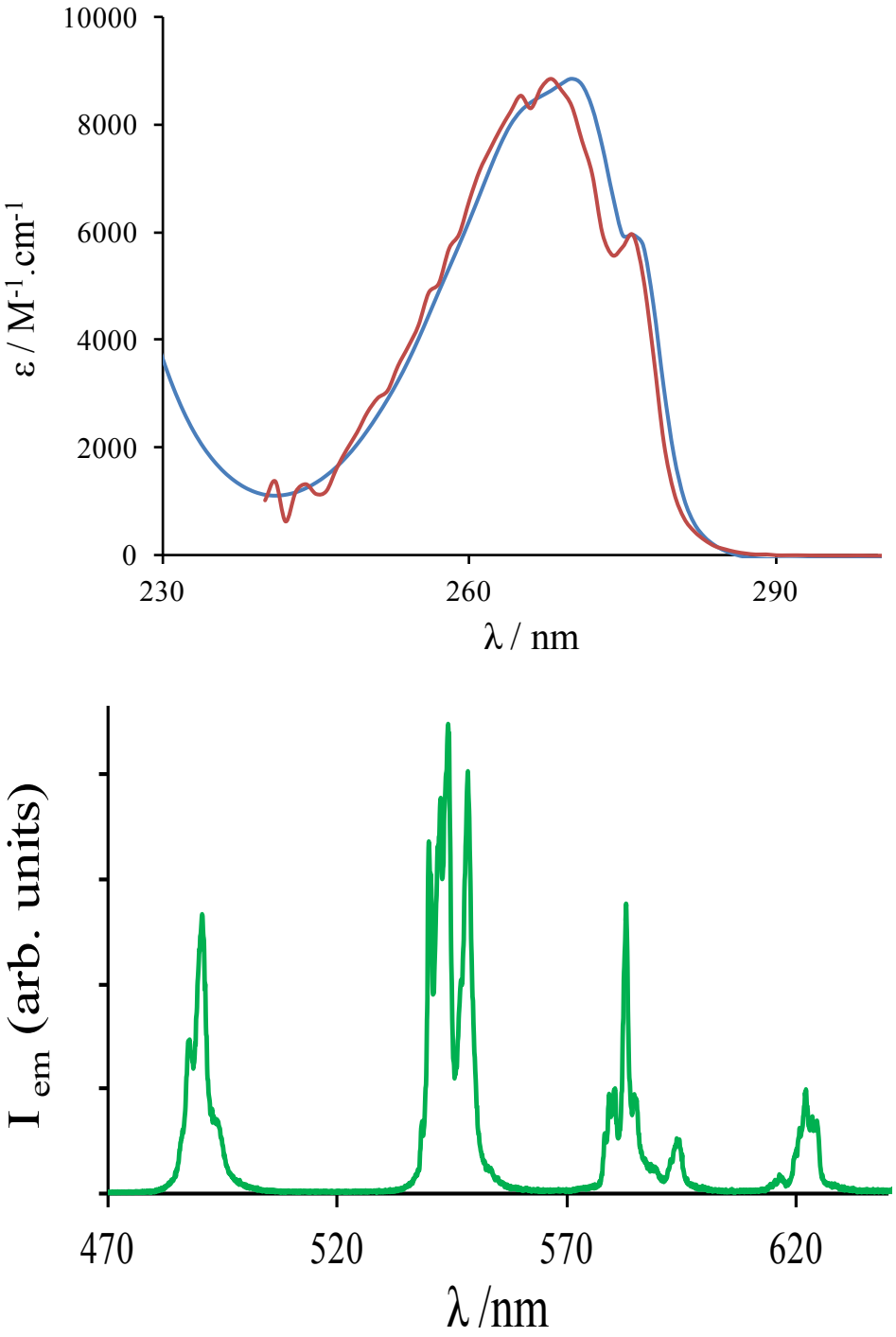


Figure S6. UV/Vis absorption spectra (blue: pH = 7.0, 8.20×10^{-5} M), excitation spectra (red: pH = 7.0, 4.09×10^{-5} M, λ_{em} = 545 nm) and high resolution emission spectra (green: pH = 7.0, 3.81×10^{-4} M, λ_{exc} = 268 nm) recorded in aqueous solution at r.t for the $[TbL^2](NO_3)_3$ complex.

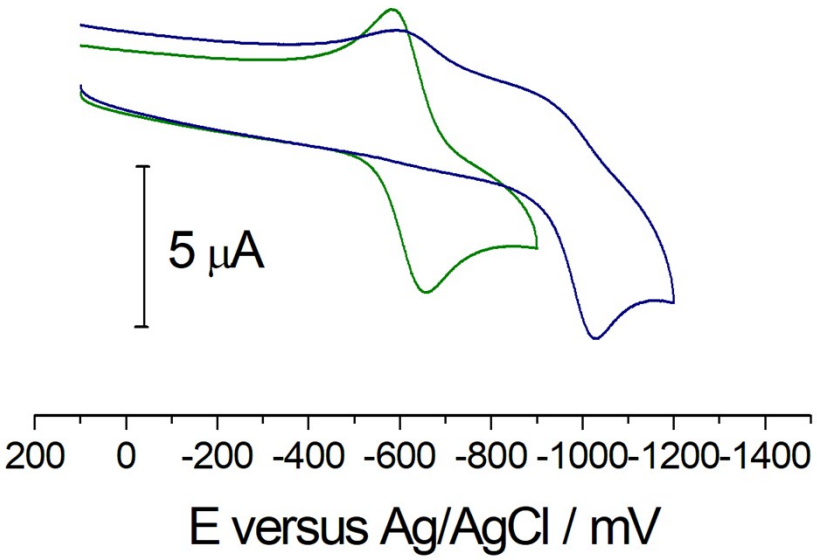


Figure S7. Cyclic voltammograms of $[EuL^1]^{3+}$ (green) and $[EuL^2]^{3+}$ (blue) recorded in 1 mM aqueous solutions (0.1 M KCl, pH 7.0) at 0.05 V/s.

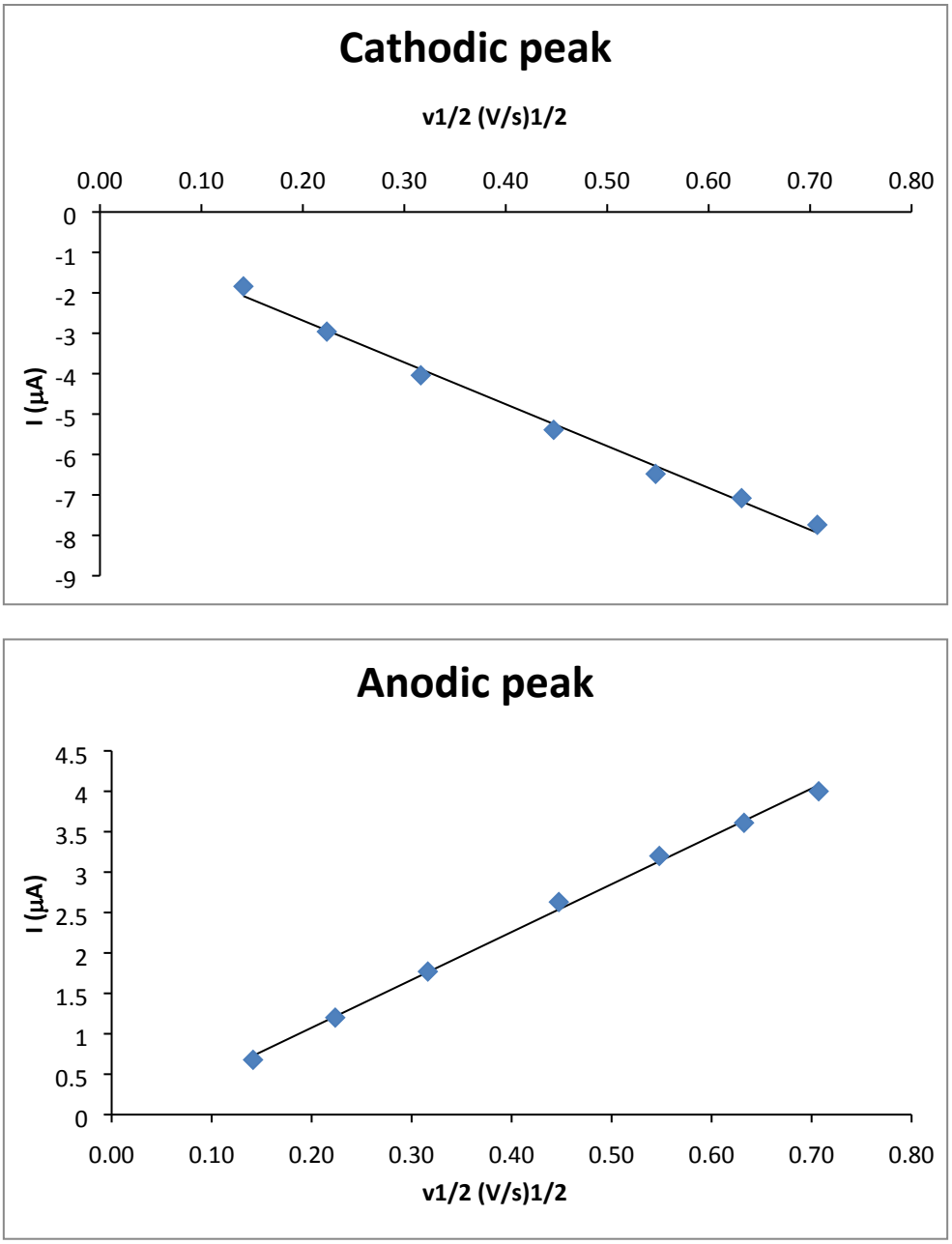


Figure S8. Plots of the anodic and cathodic currents versus the square root of the scan rate obtained from the cyclic voltammograms of $[EuL^1]^{3+}$ (0.1 M KCl, pH 7.0).

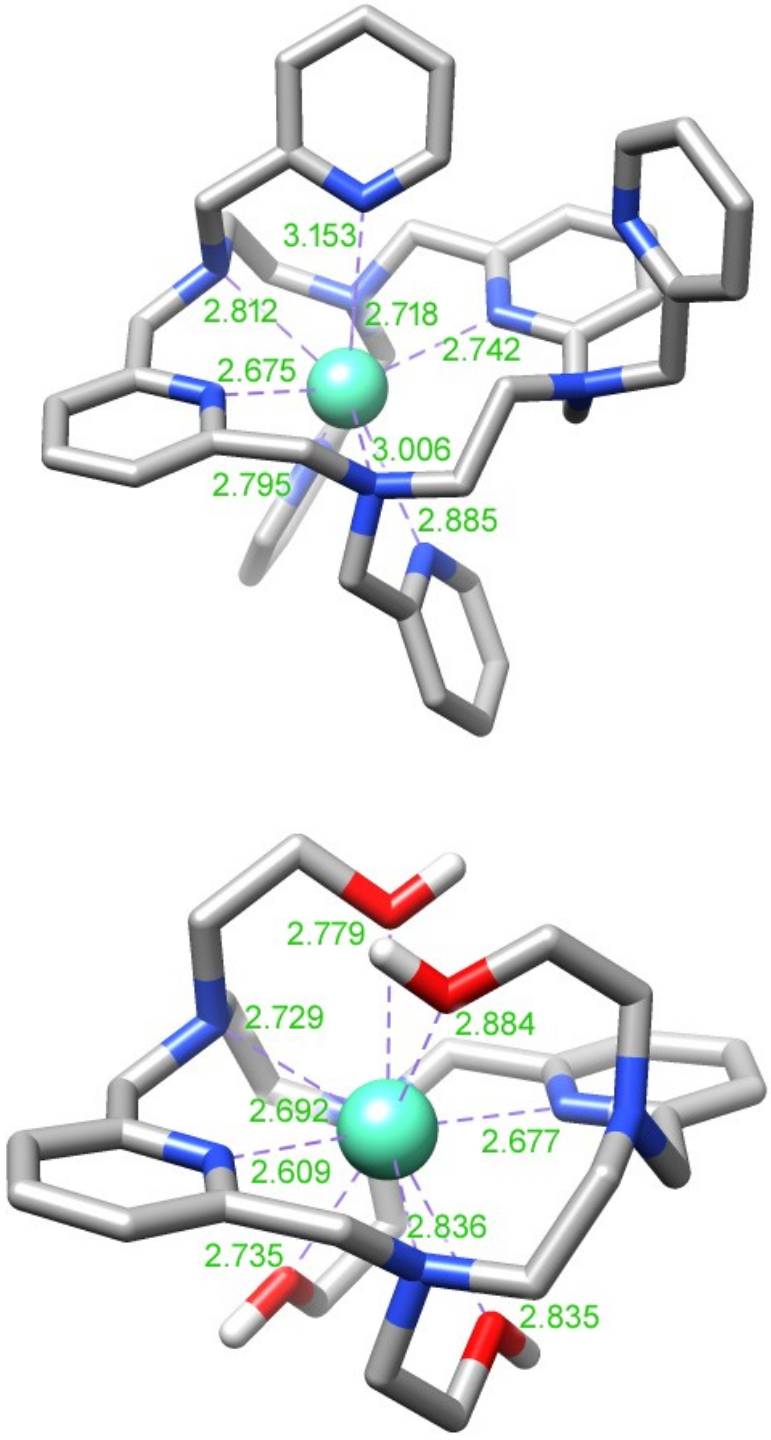
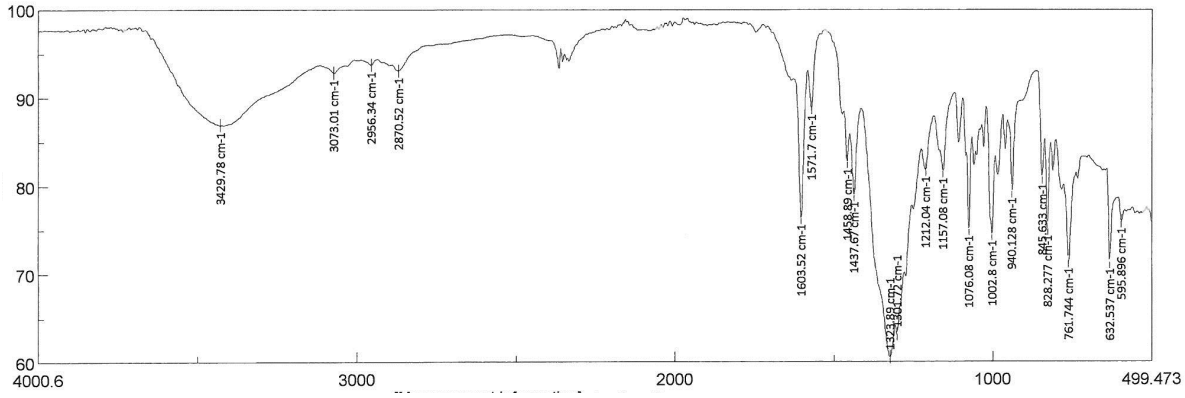


Figure S9. Structures of the $[EuL^1]^{3+}$ (top) and $[EuL^2]^{3+}$ (bottom) complexes obtained with the 46+4f^7 core definition. The numbers correspond to the bond distances of the metal coordination environment given in Å.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80
70
60
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3000
2000
1000
499.473
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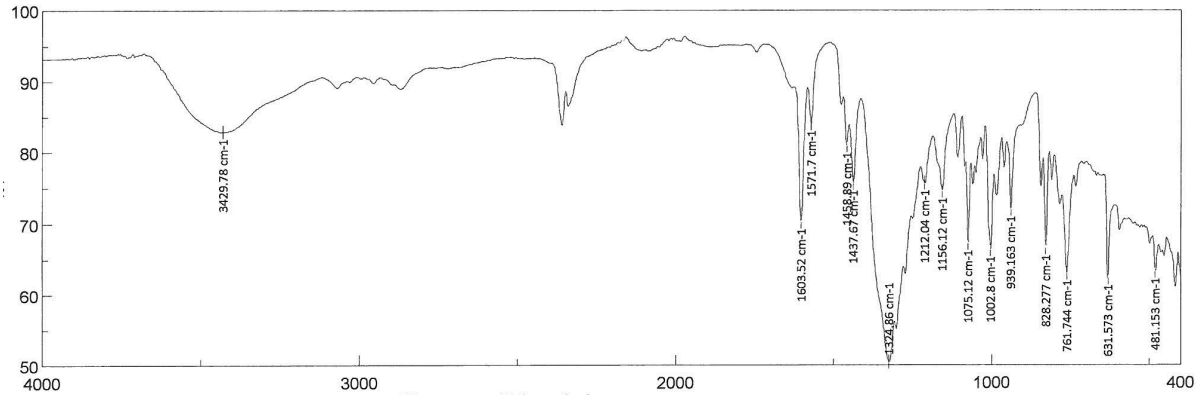
3073.01 cm-1
2956.34 cm-1
2870.52 cm-1
1603.52 cm-1
1571.7 cm-1
1458.89 cm-1
1437.67 cm-1
1323.88 cm-1
1301.72 cm-1
1212.04 cm-1
1157.08 cm-1
1076.08 cm-1
1002.8 cm-1
940.128 cm-1
845.633 cm-1
828.277 cm-1
761.744 cm-1
632.537 cm-1
595.896 cm-1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90
80
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3429.78 cm-1
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1458.89 cm-1
1437.67 cm-1
1374.86 cm-1
1212.04 cm-1
1156.12 cm-1
1075.12 cm-1
1002.8 cm-1
939.163 cm-1
828.277 cm-1
761.744 cm-1
631.573 cm-1
481.153 cm-1

Figure S10. IR spectrum of $[EuL^1](NO_3)_3 \cdot 4H_2O$.

Figure S11. IR spectrum of $[GdL^1](NO_3)_3 \cdot 6H_2O$.

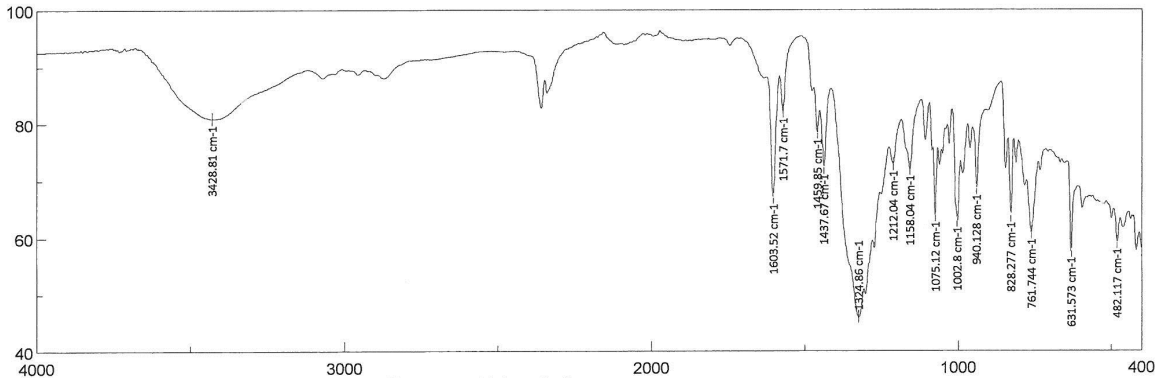

Figure S12. IR spectrum of $[TbL^1](NO_3)_3 \cdot 4H_2O$.

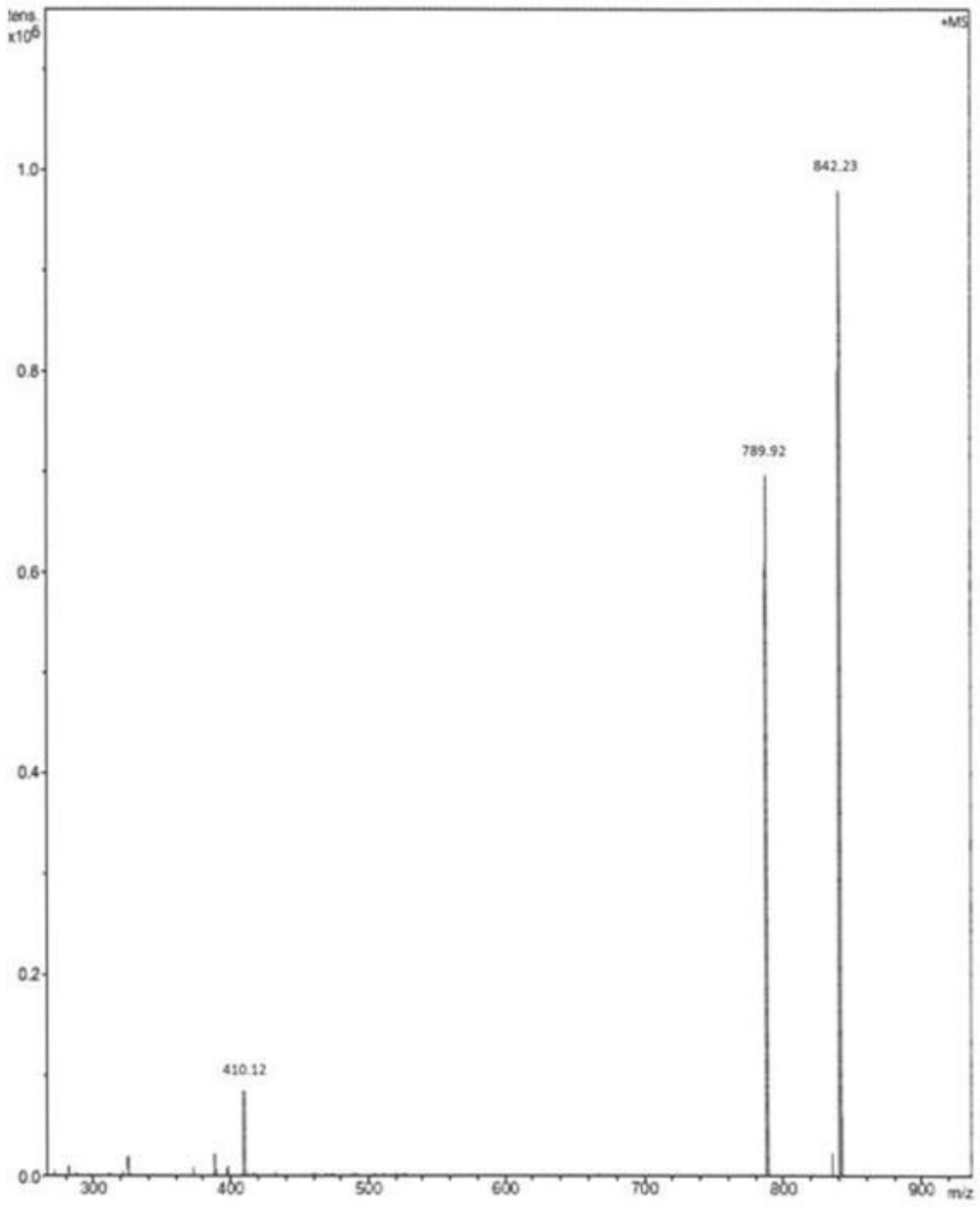

Figure S13. MS-ESI of $[EuL^1](NO_3)_3 \cdot 4H_2O$.

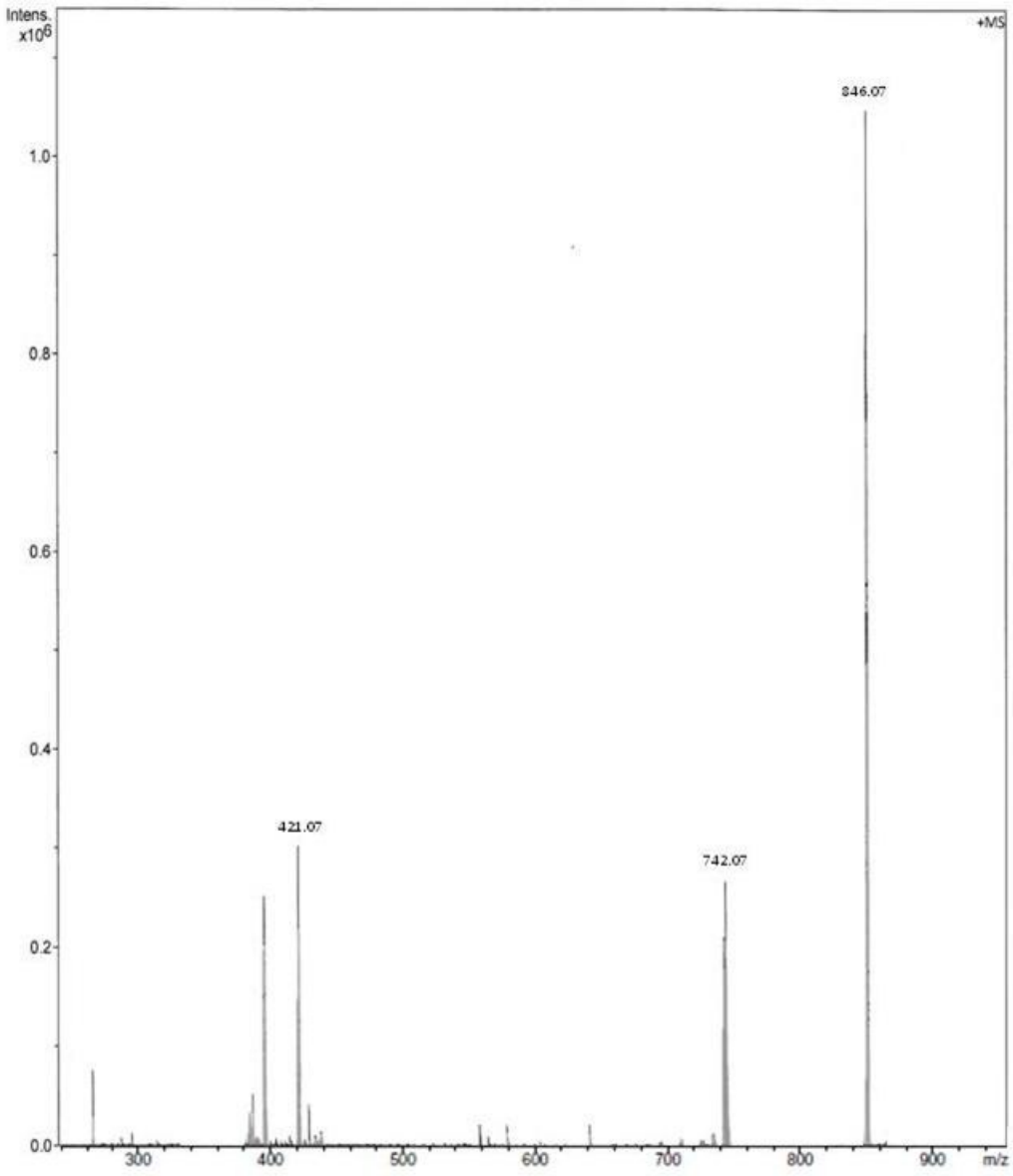

Figure S14. MS-ESI of $[GdL^1](NO_3)_3 \cdot 6H_2O$.

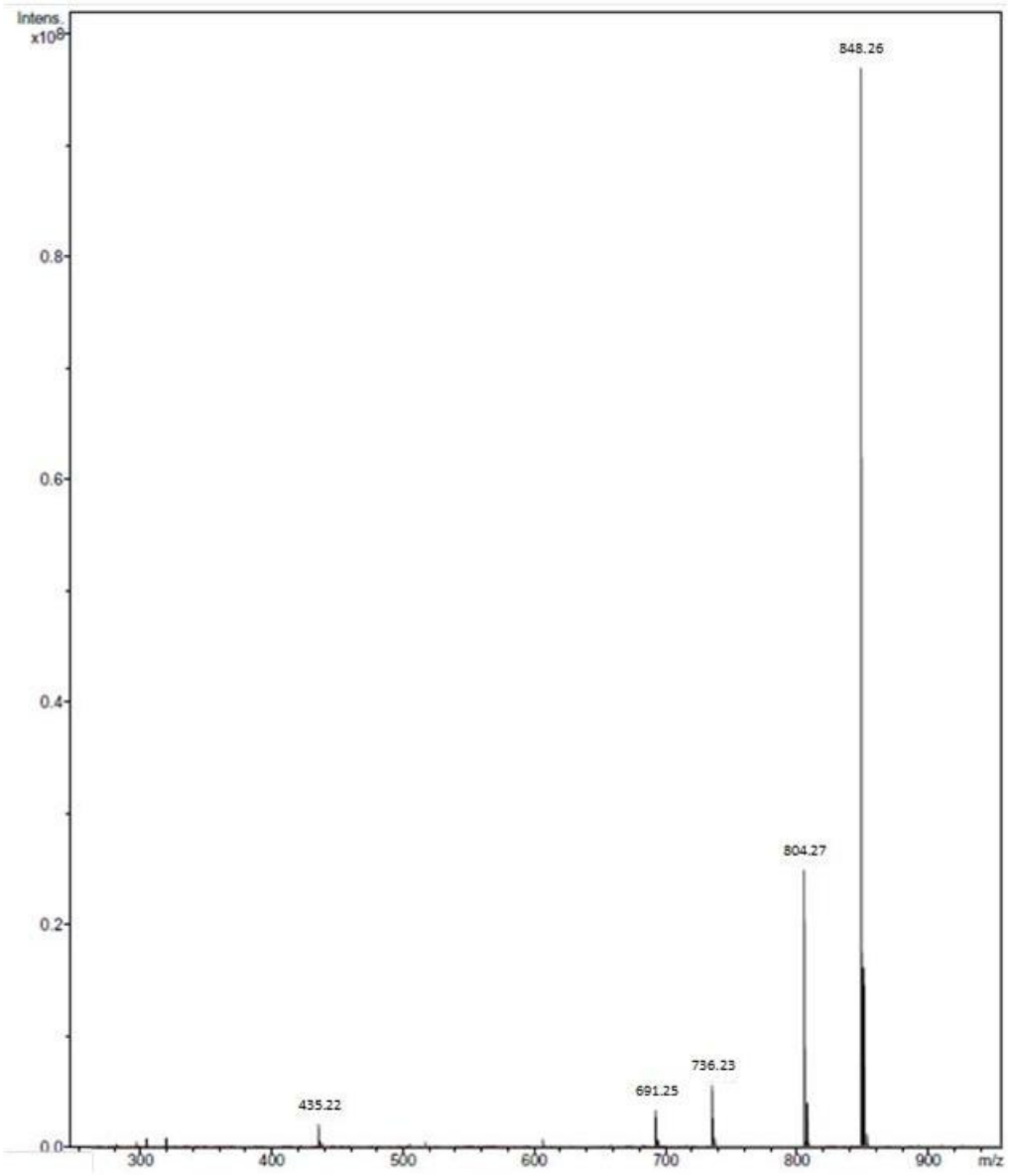

Figure S15. MS-ESI of $[TbL^1](NO_3)_3 \cdot 4H_2O$

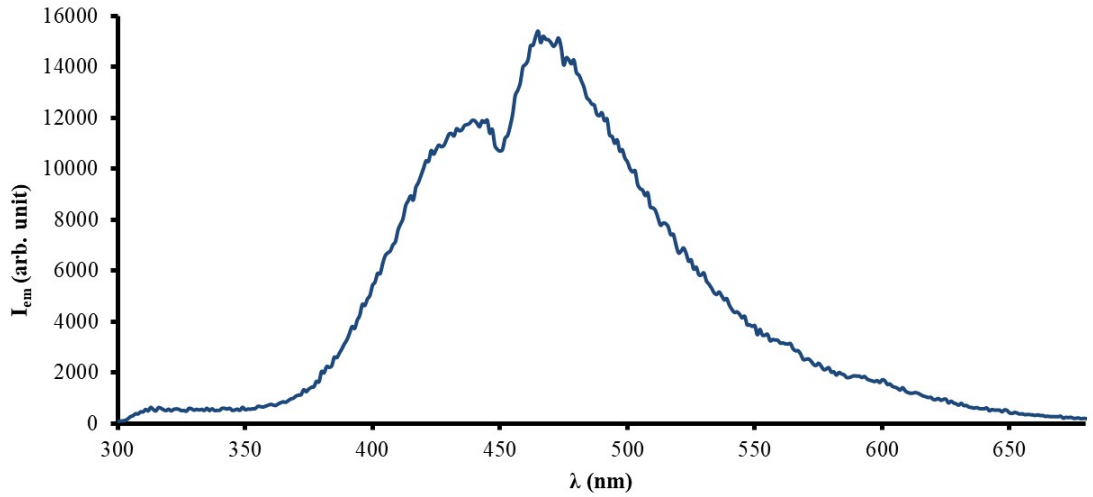

Figure S16. Phosphorescence emission spectra (λ_{exc} = 265 nm) recorded for [GdL^1] in a 90/10 H_2O/glycerol mixture frozen solution at 77.5K (1.63 mM, pH =7.0).

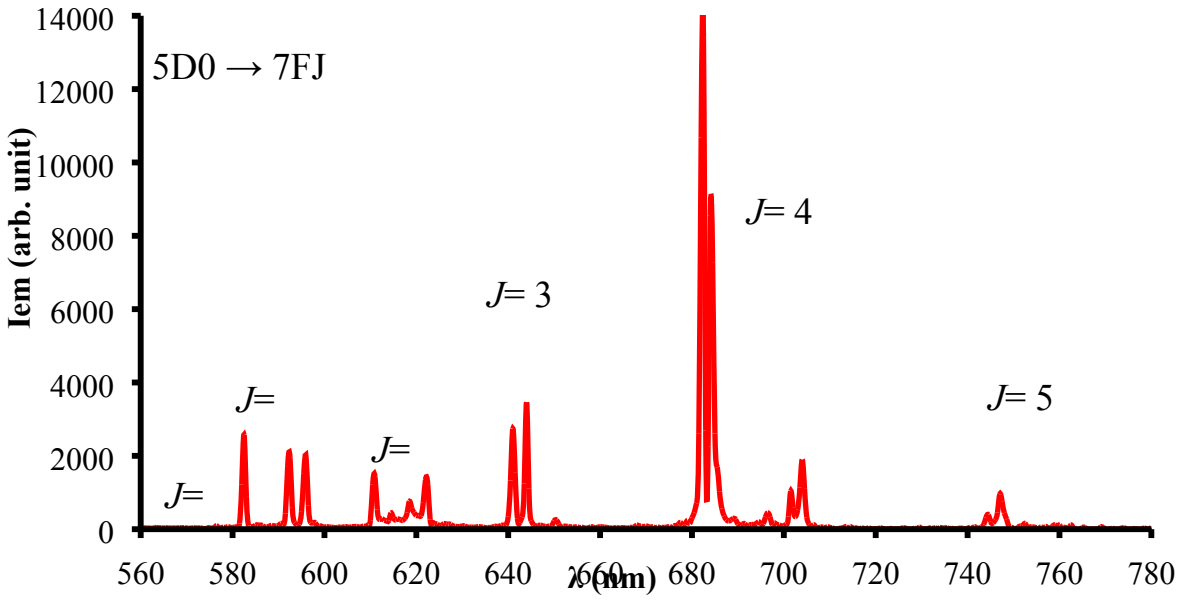

Figure S17. High resolution emission spectra (λ_{exc} = 265 nm, emission slits = 0.2 nm, increment = 0.5 nm) recorded for [EuL^1] in a 90/10 H_2O/glycerol frozen solution at 77.5 K (9.83×10^{-4}M, pH =7.0).

Table S1. Optimized Cartesian coordinates obtained for $[EuL^1]^{3+}$ using the 46+4f^6 core definition (0 Imaginary Frequencies, singlet).

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	6	0	-0.154565	-3.286343	-1.156370
2	6	0	-0.178840	-4.681826	-1.188827
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8	6	0	-0.676913	0.339063	3.480910
9	6	0	-0.223246	2.486338	2.434980
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13	6	0	0.178848	4.681798	-1.188927
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21	6	0	4.411067	0.045510	2.266876
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23	6	0	4.343749	2.297136	1.451173
24	6	0	3.030521	2.057257	1.058636
25	6	0	-2.357580	1.401755	2.129099
26	6	0	-3.088413	0.111691	1.844836
27	6	0	-4.411061	-0.045468	2.266904
28	6	0	-5.058473	-1.260373	2.051422
29	6	0	-4.343738	-2.297113	1.451256
30	6	0	-3.030513	-2.057239	1.058706
31	6	0	2.357619	1.401647	-2.129105
32	6	0	3.088419	0.111567	-1.844826
33	6	0	4.411062	-0.045632	-2.266893
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Sum of electronic and thermal Energies= -2210.172676
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Sum of electronic and thermal Free Energies = -2210.288924

Table S2. Optimized Cartesian coordinates obtained for $[EuL^1]^{3+}$ using the 46+4f^7 core definition (0 Imaginary Frequencies, doublet).

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	6	0	-0.877874	-0.122466	3.652416
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64	1	0	1.286267	2.010099	-4.770838
65	1	0	3.080831	0.309294	-5.135948
66	1	0	3.329117	-1.556881	-3.505759
67	1	0	0.817617	-2.061629	-0.722393
68	1	0	1.929215	-2.924846	-1.799510
69	1	0	2.247101	-0.486606	1.160620
70	1	0	3.506483	-1.602493	1.678080
71	1	0	1.938234	-2.866687	2.708348
72	1	0	1.275438	-3.307351	1.141585

73	1	0	0.559864	-1.624183	4.201136
74	1	0	1.195680	-0.306870	3.208180
75	1	0	-0.345693	2.951676	2.545142
76	1	0	-0.824086	4.495740	1.831655
77	1	0	1.150237	5.601331	1.215515
78	1	0	3.375278	5.594186	0.064866
79	1	0	4.204220	3.428669	-0.914272
80	1	0	2.794458	1.402920	-0.688779
81	1	0	-2.776063	1.515138	-3.848701
82	1	0	-1.743678	0.137713	-3.449267
83	1	0	-4.896168	0.373338	-4.118284
84	1	0	-6.764702	-0.908757	-3.059521
85	1	0	-6.449139	-1.797026	-0.726809
86	1	0	-4.271553	-1.369018	0.421589
87	1	0	4.246047	-3.416444	-0.149986
88	1	0	4.209802	-2.536371	-1.679622
89	1	0	6.642748	-3.112387	0.387876
90	1	0	8.456728	-1.523522	1.067251
91	1	0	7.995416	0.945607	0.952716
92	1	0	5.754158	1.707131	0.169082
93	1	0	-1.741681	-2.277075	2.671051
94	1	0	-0.572323	-3.544467	3.046972
95	1	0	-1.465071	-5.446875	1.914885
96	1	0	-2.205947	-6.527933	-0.216276
97	1	0	-2.356441	-5.114289	-2.293924
98	1	0	-1.754246	-2.698758	-2.131330
99	63	0	-0.968471	0.107387	0.082082

E(UTPSSh) = -2204.983065 Hartree
Zero-point correction = 0.827886
Thermal correction to Energy = 0.873416
Thermal correction to Enthalpy = 0.874360
Thermal correction to Gibbs Free Energy = 0.747147
Sum of electronic and zero-point Energies = -2204.155179
Sum of electronic and thermal Energies = -2204.109649
Sum of electronic and thermal Enthalpies = -2204.108704
Sum of electronic and thermal Free Energies = -2204.235918

Table S3. Optimized Cartesian coordinates obtained for $[EuL^2]^{3+}$ using the 46+4f^6 core definition (0 Imaginary Frequencies, singlet).

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	63	0	-0.000040	-0.000164	-0.000105
2	7	0	-2.590305	0.000071	0.000509
3	7	0	-1.139742	2.238709	0.958259
4	7	0	1.139940	2.238546	-0.958485
5	7	0	2.590321	0.000017	-0.000309
6	7	0	1.139985	-2.238564	0.958239
7	7	0	-1.140181	-2.238711	-0.957908
8	8	0	0.900072	1.072698	2.138207
9	8	0	-0.899814	1.072168	-2.138591
10	8	0	-0.899127	-1.071581	2.139072
11	8	0	0.899262	-1.072844	-2.138704
12	6	0	-3.276370	-1.146462	-0.219175
13	6	0	-4.671520	-1.176783	-0.245714
14	1	0	-5.189067	-2.108694	-0.443067
15	6	0	-5.376988	0.000317	0.000034
16	1	0	-6.461636	0.000411	-0.000142
17	6	0	-4.671395	1.177283	0.245995

18	1	0	-5.188838	2.109297	0.443138
19	6	0	-3.276227	1.146719	0.219909
20	6	0	-2.482122	2.427966	0.353758
21	1	0	-2.339667	2.840959	-0.649437
22	1	0	-3.064105	3.165563	0.921962
23	6	0	-0.300263	3.446605	0.697287
24	1	0	0.495196	3.472380	1.441317
25	1	0	-0.894063	4.359998	0.834835
26	6	0	0.300582	3.446542	-0.697575
27	1	0	-0.494913	3.472369	-1.441559
28	1	0	0.894446	4.359881	-0.835196
29	6	0	2.482377	2.427834	-0.354149
30	1	0	2.340043	2.841213	0.648902
31	1	0	3.064387	3.165182	-0.922647
32	6	0	3.276355	1.146539	-0.219984
33	6	0	4.671525	1.176981	-0.246123
34	1	0	5.189032	2.108927	-0.443415
35	6	0	5.377021	-0.000016	-0.000041
36	1	0	6.461669	-0.000026	0.000083
37	6	0	4.671445	-1.177010	0.245892
38	1	0	5.188906	-2.108958	0.443296
39	6	0	3.276293	-1.146545	0.219477
40	6	0	2.482244	-2.427809	0.353467
41	1	0	2.339583	-2.840842	-0.649681
42	1	0	3.064340	-3.165369	0.921602
43	6	0	0.300540	-3.446558	0.697583
44	1	0	-0.494741	-3.472367	1.441794
45	1	0	0.894422	-4.359909	0.835045
46	6	0	-0.300705	-3.446668	-0.697112
47	1	0	0.494553	-3.472534	-1.441354
48	1	0	-0.894612	-4.360019	-0.834442
49	6	0	-2.482393	-2.427793	-0.352933
50	1	0	-2.339625	-2.840595	0.650293
51	1	0	-3.064583	-3.165469	-0.920819
52	6	0	-1.283235	2.049857	2.427051
53	1	0	-1.958327	1.208245	2.585639
54	1	0	-1.743075	2.932007	2.893403
55	6	0	0.071482	1.791815	3.088030
56	6	0	1.283324	2.049307	-2.427279
57	1	0	1.957940	1.207273	-2.585661
58	1	0	1.743605	2.931103	-2.893863
59	6	0	-0.071485	1.791856	-3.088144
60	6	0	1.283833	-2.049244	2.427000
61	1	0	1.958383	-1.207113	2.585115
62	1	0	1.744306	-2.930998	2.893465
63	6	0	-0.070757	-1.791808	3.088253
64	6	0	-1.284111	-2.049861	-2.426684
65	1	0	-1.958963	-1.208015	-2.585072
66	1	0	-1.744382	-2.931877	-2.892852
67	6	0	0.070469	-1.792311	-3.088056
68	1	0	0.060718	1.201616	-3.998028
69	1	0	-0.577154	2.723788	-3.352288
70	1	0	-0.062086	-1.201850	-3.997742
71	1	0	0.575987	-2.724208	-3.352604
72	1	0	0.061743	-1.201891	3.998306
73	1	0	-0.576598	-2.723705	3.352181
74	1	0	-0.061011	1.200886	3.997420
75	1	0	0.577168	2.723503	3.352970
76	1	0	-1.805372	-1.026381	2.479923
77	1	0	1.806714	1.029089	2.478215
78	1	0	1.805485	-1.027979	-2.479664
79	1	0	-1.806098	1.026930	-2.479339

E(RTPSSh) = -1680.71908852 Hartree
Zero-point correction = 0.689700
Thermal correction to Energy = 0.725059

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Thermal correction to Enthalpy = 0.726003
Thermal correction to Gibbs Free Energy = 0.628074
Sum of electronic and zero-point Energies = -1680.029388
Sum of electronic and thermal Energies = -1679.994030
Sum of electronic and thermal Enthalpies = -1679.993085
Sum of electronic and thermal Free Energies = -1680.091015
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Table S4. Optimized Cartesian coordinates obtained for $[EuL^4]^{3+}$ using the 46+4f^7 core definition (0 Imaginary Frequencies, doublet).

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	63	0	0.000022	0.000208	-0.000017
2	7	0	2.666202	0.000111	0.000344
3	7	0	1.277272	-2.377418	0.907338
4	7	0	-1.276092	-2.377165	-0.907392
5	7	0	-2.666190	-0.000432	-0.000321
6	7	0	-1.276903	2.376656	0.907288
7	7	0	1.275542	2.376353	-0.906449
8	8	0	-0.787639	-1.261347	2.296231
9	8	0	0.788256	-1.260541	-2.296171
10	8	0	0.786984	1.260733	2.297161
11	8	0	-0.787659	1.260645	-2.296816
12	6	0	3.345223	1.159608	-0.122718
13	6	0	4.741760	1.196254	-0.144745
14	1	0	5.262118	2.140053	-0.264222
15	6	0	5.446079	0.000819	0.000010
16	1	0	6.530852	0.001107	-0.000122
17	6	0	4.742446	-1.195021	0.144906
18	1	0	5.263324	-2.138559	0.264186
19	6	0	3.345921	-1.158998	0.123188
20	6	0	2.550207	-2.456434	0.165583
21	1	0	2.314603	-2.752865	-0.860716
22	1	0	3.183295	-3.245741	0.596859
23	6	0	0.386914	-3.521931	0.672155
24	1	0	-0.323593	-3.577006	1.493839
25	1	0	0.965756	-4.456305	0.674892
26	6	0	-0.385881	-3.521849	-0.672361
27	1	0	0.324703	-3.576869	-1.493997
28	1	0	-0.964604	-4.456296	-0.675217
29	6	0	-2.549285	-2.456935	-0.166103
30	1	0	-2.313926	-2.753511	0.860215
31	1	0	-3.182068	-3.246309	-0.597708
32	6	0	-3.345444	-1.159771	-0.123550
33	6	0	-4.741968	-1.196232	-0.145607
34	1	0	-5.262486	-2.139926	-0.265211
35	6	0	-5.446071	-0.000683	-0.000665
36	1	0	-6.530844	-0.000783	-0.000793
37	6	0	-4.742221	1.194995	0.144429
38	1	0	-5.262936	2.138600	0.263886
39	6	0	-3.345685	1.158790	0.122712
40	6	0	-2.549730	2.456074	0.165360
41	1	0	-2.313892	2.752406	-0.860918
42	1	0	-3.182846	3.245466	0.596454
43	6	0	-0.386768	3.521706	0.672605
44	1	0	0.323791	3.576370	1.494293
45	1	0	-0.965719	4.456031	0.676153
46	6	0	0.385757	3.521702	-0.671694
47	1	0	-0.324931	3.576569	-1.493278
48	1	0	0.964641	4.456067	-0.675190

49	6	0	2.548787	2.456602	-0.165223
50	1	0	2.313381	2.752932	0.861163
51	1	0	3.181502	3.246137	-0.596651
52	6	0	1.482211	-2.050951	2.336557
53	1	0	2.035060	-1.110416	2.371923
54	1	0	2.111384	-2.817020	2.815008
55	6	0	0.180208	-1.934830	3.124086
56	6	0	-1.481222	-2.051453	-2.336794
57	1	0	-2.034795	-1.111355	-2.372542
58	1	0	-2.109684	-2.818144	-2.815183
59	6	0	-0.179164	-1.934500	-3.124161
60	6	0	-1.482705	2.051092	2.336579
61	1	0	-2.036104	1.110875	2.372212
62	1	0	-2.111585	2.817689	2.814592
63	6	0	-0.181008	1.934532	3.124612
64	6	0	1.481685	2.052381	-2.336125
65	1	0	2.035947	1.112700	-2.372624
66	1	0	2.109739	2.819942	-2.813674
67	6	0	0.179980	1.935188	-3.124117
68	1	0	-0.375202	-1.363775	-4.036734
69	1	0	0.205621	-2.917828	-3.412932
70	1	0	0.376505	1.364854	-4.036840
71	1	0	-0.205028	2.918493	-3.412679
72	1	0	-0.377354	1.363860	4.037161
73	1	0	0.203380	2.917993	3.413451
74	1	0	0.376104	-1.364053	4.036657
75	1	0	-0.203969	-2.918396	3.412848
76	1	0	1.615634	1.193016	2.795044
77	1	0	-1.616344	-1.193304	2.793984
78	1	0	-1.616125	1.192231	-2.794906
79	1	0	1.616829	-1.191621	-2.794020

E(UTPSSh) = -1674.6372751 Hartree
Zero-point correction = 0.685405
Thermal correction to Energy = 0.722053
Thermal correction to Enthalpy = 0.722998
Thermal correction to Gibbs Free Energy = 0.620242
Sum of electronic and zero-point Energies = -1673.951870
Sum of electronic and thermal Energies = -1673.915222
Sum of electronic and thermal Enthalpies = -1673.914278
Sum of electronic and thermal Free Energies = -1674.017033