Supporting Information for:

Magnetic Anisotropies in Rhombic Ln(III) Complexes Do Not Conform to Bleaney's Theory

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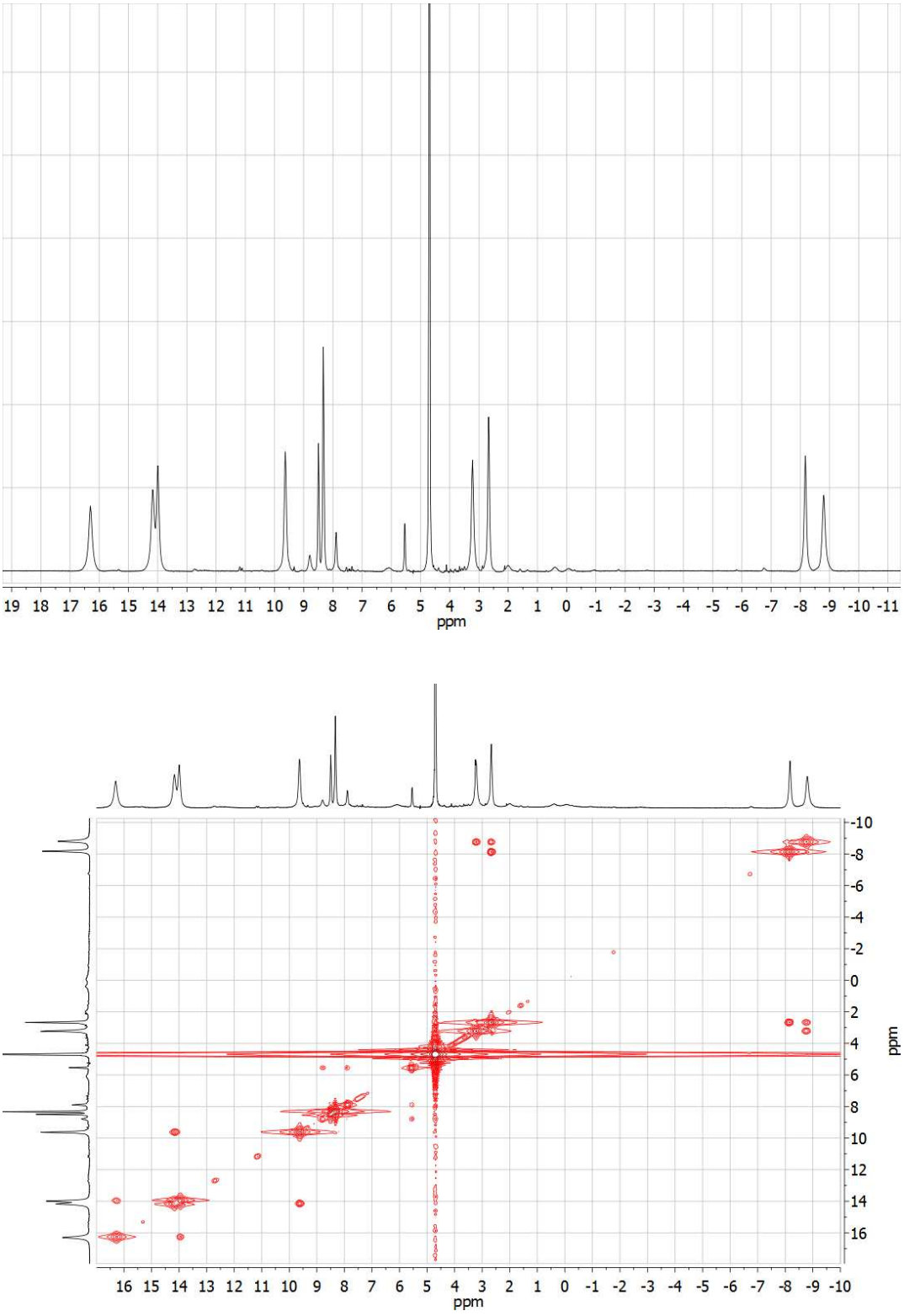

Figure S1. ^{1}H (400 MHz, 25 ºC, top) and ^{1}H-^{1}H COSY (400 MHz, 25 ºC, bottom) NMR spectra of $[CeL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

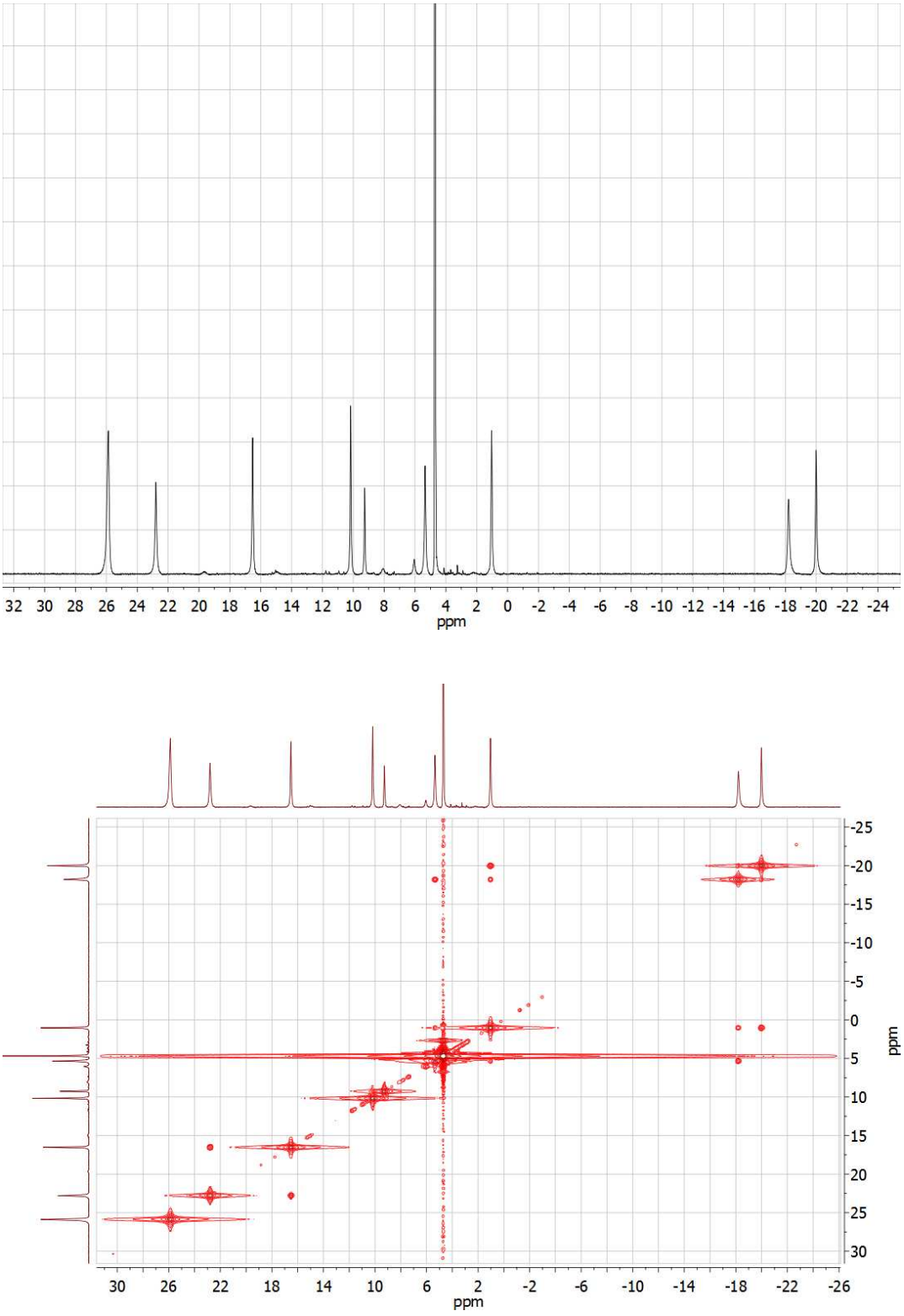

Figure S2. ^{1}H (400 MHz, 25 ºC, top) and ^{1}H-^{1}H COSY (400 MHz, 25 ºC, bottom) NMR spectra of $[PrL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

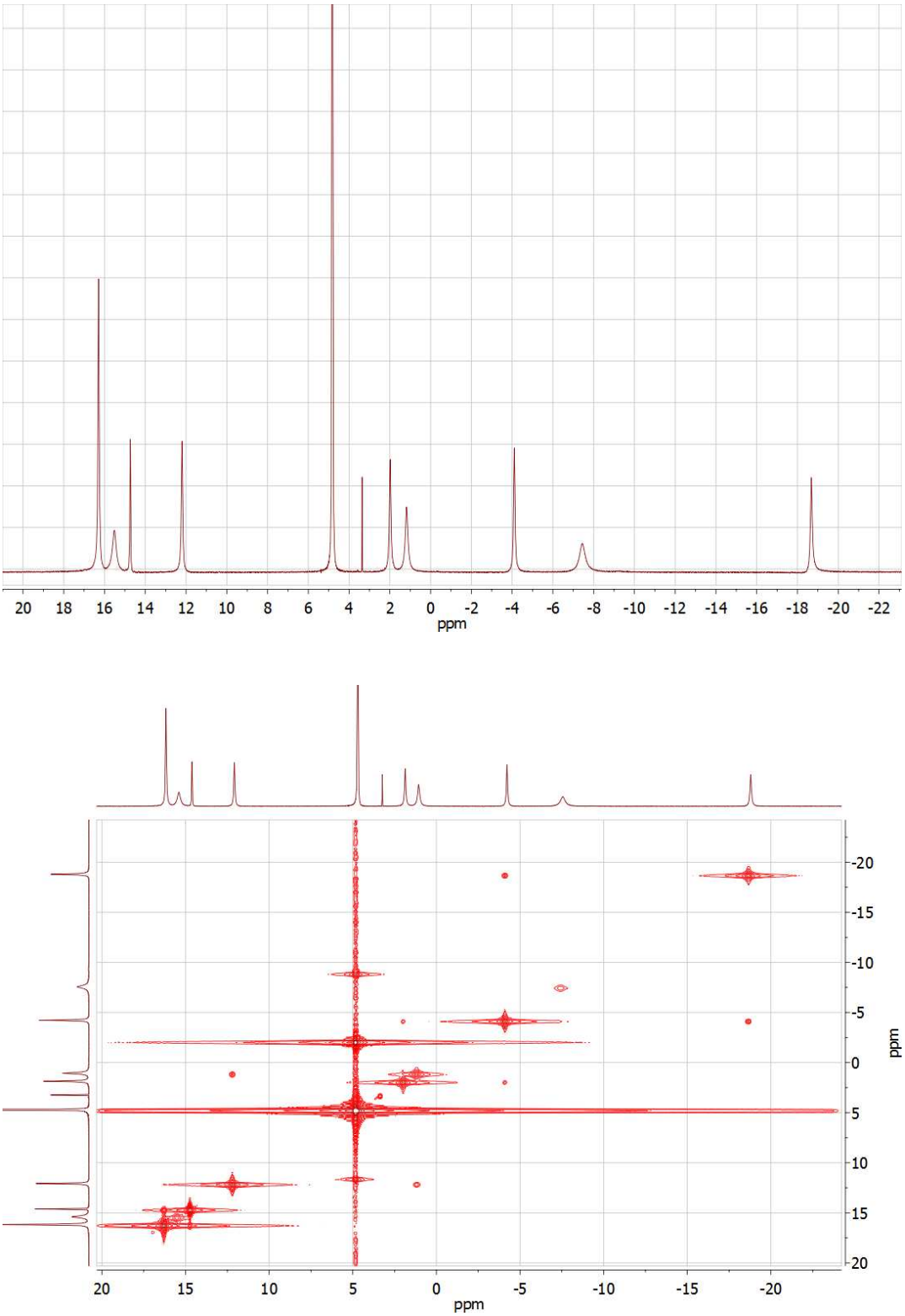

Figure S3. ^{1}H (400 MHz, 25 ºC, top) and ^{1}H-^{1}H COSY (400 MHz, 25 ºC, bottom) NMR spectra of $[NdL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

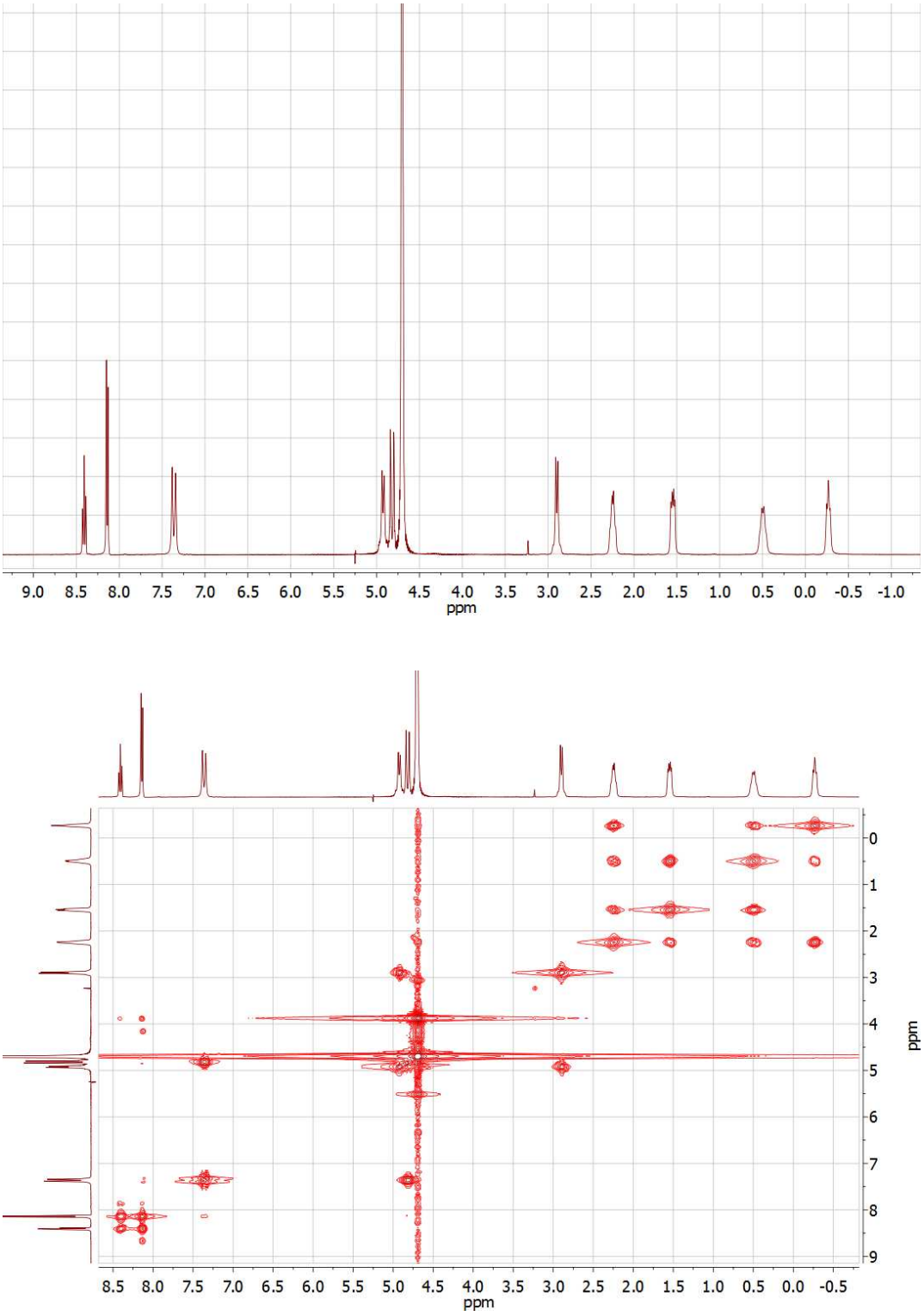

Figure S4. ^{1}H (400 MHz, 25 ºC, top) and ^{1}H-^{1}H COSY (400 MHz, 25 ºC, bottom) NMR spectra of $[SmL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

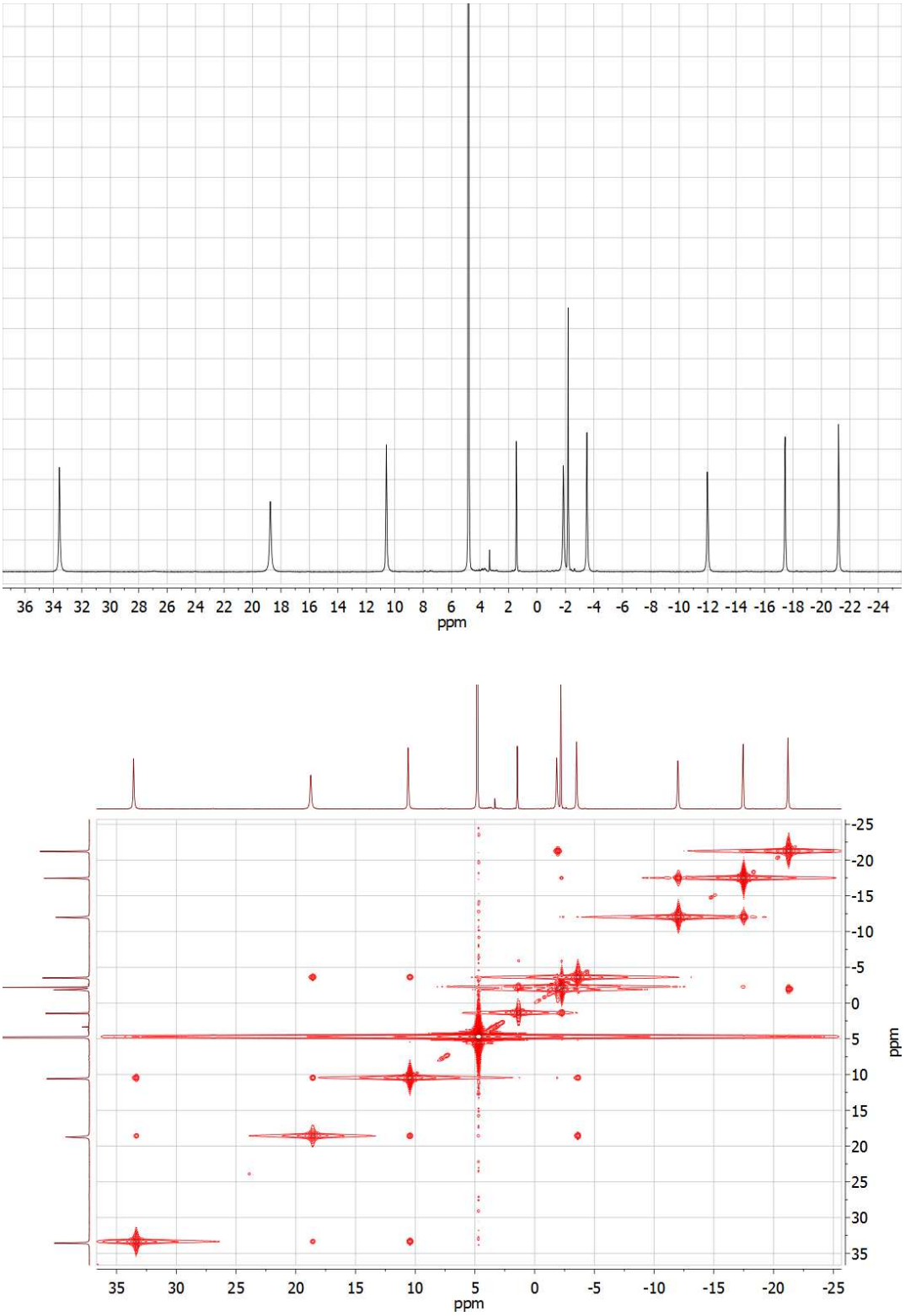

Figure S5. ^{1}H (400 MHz, 25 ºC, top) and ^{1}H-^{1}H COSY (400 MHz, 25 ºC, bottom) NMR spectra of $[EuL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

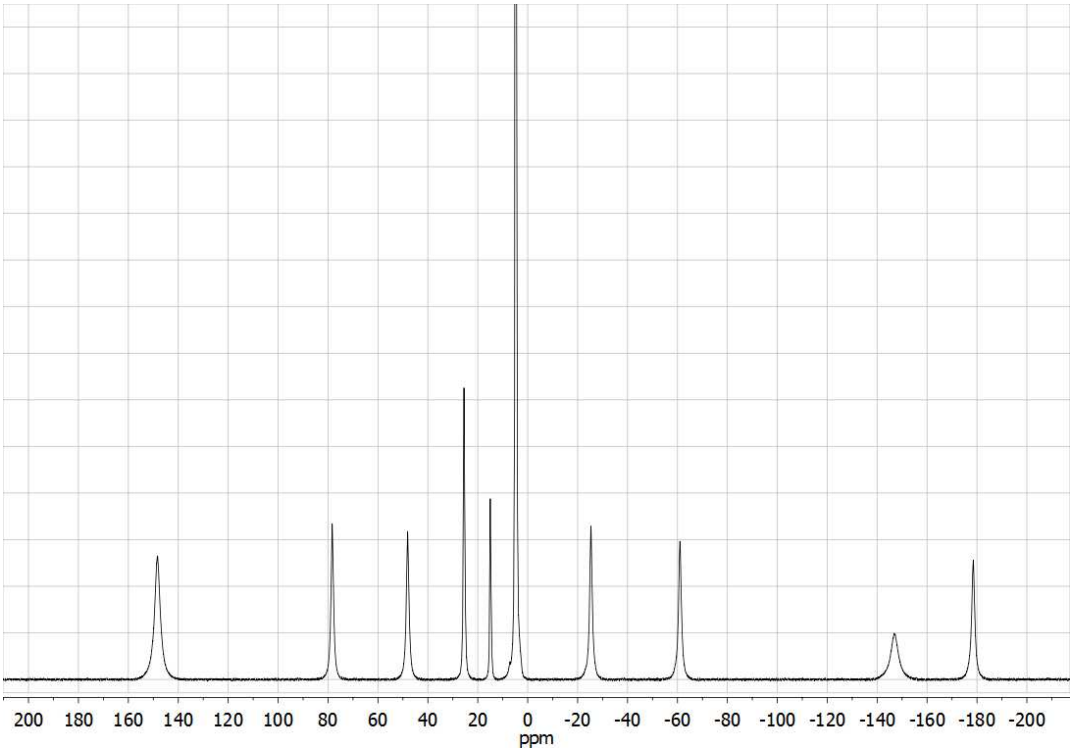

Figure S6. ^{1}H (400 MHz, 25 ºC) NMR spectrum of $[TbL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

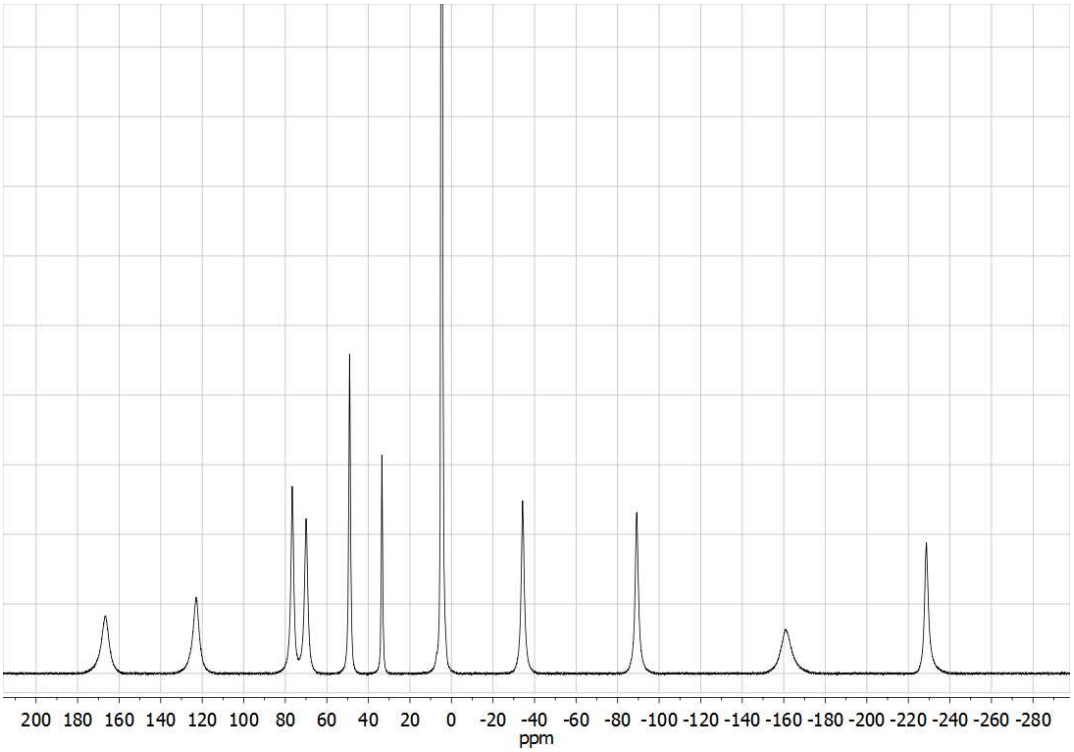

Figure S7. ^{1}H (400 MHz, 25 ºC, top) NMR spectrum of $[DyL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

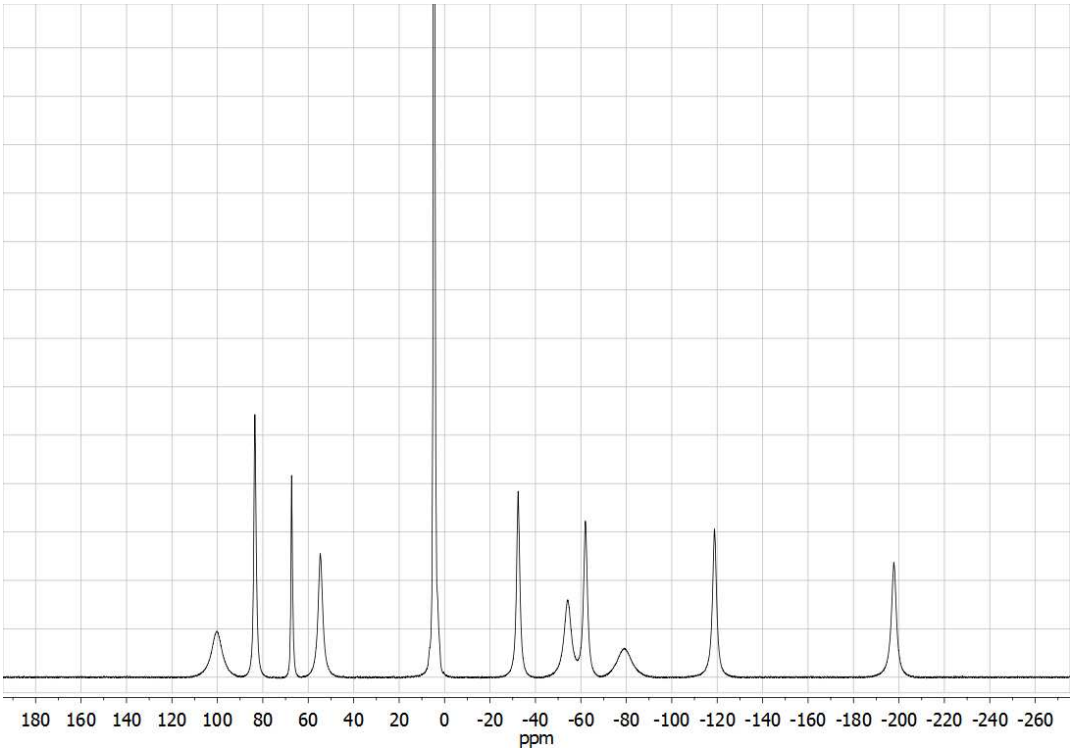

Figure S8. ^{1}H (400 MHz, 25 ºC, top) NMR spectrum of $[HoL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

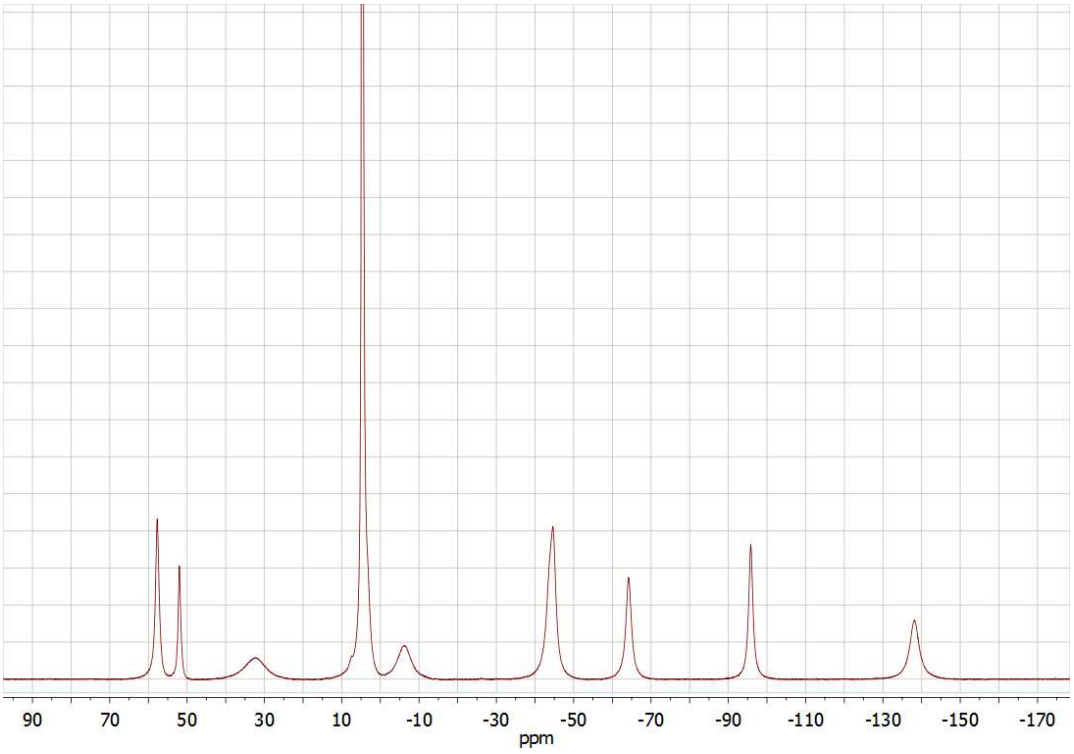

Figure S9. ^{1}H (400 MHz, 25 ºC, top) NMR spectrum of $[ErL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

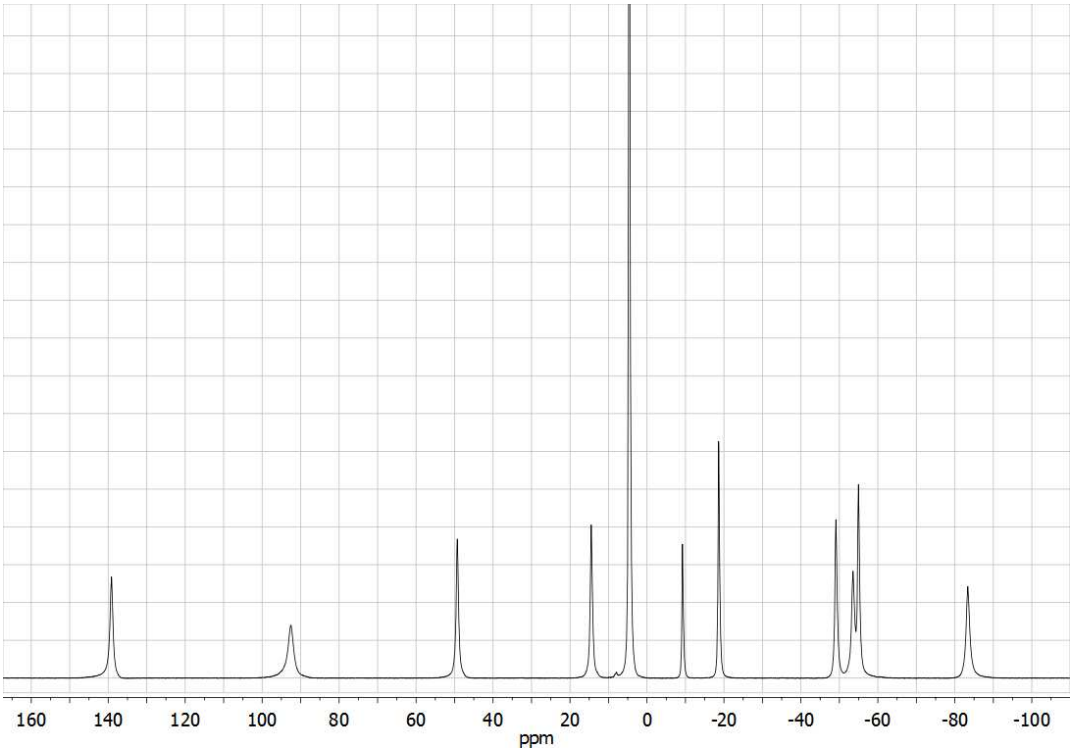

Figure S10. ^{1}H (400 MHz, 25 ºC, top) NMR spectrum of $[TmL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

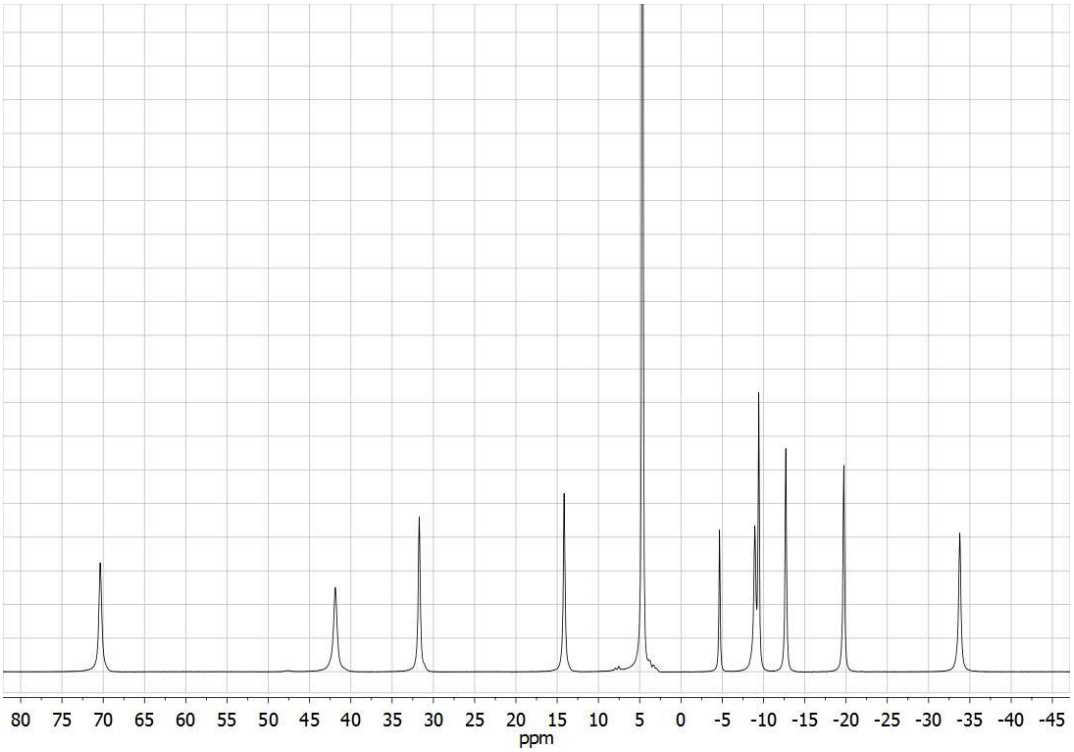

Figure S11. ^{1}H (400 MHz, 25 ºC, top) NMR spectrum of $[YbL^{1}]^{3+}$ recorded in D_2O solution (pH= 7.0).

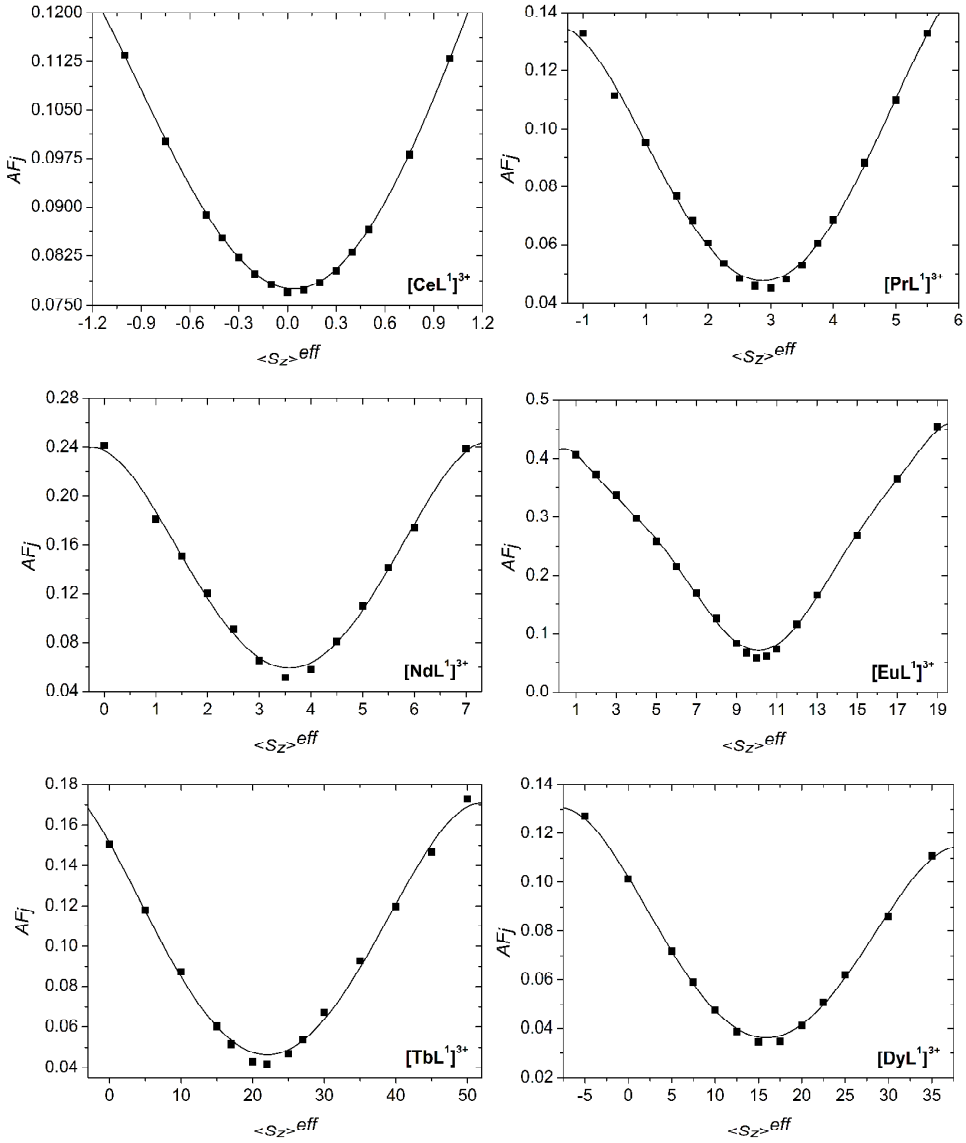

Figure S12. Plot of the agreement factor AF_j versus the effective $\langle S_z \rangle$ value used in the analysis of the ^{1}H NMR paramagnetic shifts of $[CeL^1]^{3+}$, $[PrL^1]^{3+}$, $[NdL^1]^{3+}$, $[EuL^1]^{3+}$, $[TbL^1]^{3+}$ and $[DyL^1]^{3+}$. The solid lines represent the fit of the data with minima at $\langle S_z \rangle^{eff}$ of -0.037 (Ce), -2.37 (Pr), -3.58 (Nd), 10.06 (Eu), 22.01 (Tb) and 15.88 (Dy).

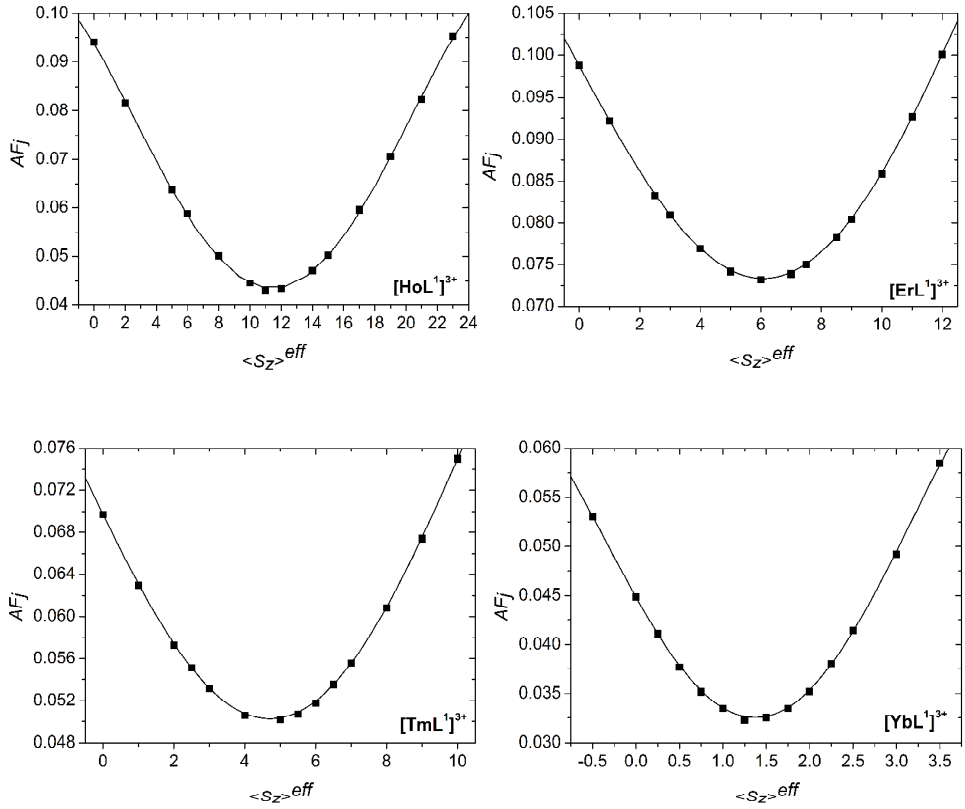

Figure S13. Plot of the agreement factor AF_j versus the effective $\langle S_z \rangle$ value used in the analysis of the ^{1}H NMR paramagnetic shifts of $[HoL^1]^{3+}$, $[ErL^1]^{3+}$, $[TmL^1]^{3+}$ and $[YbL^1]^{3+}$. The solid lines represent the fit of the data with minima at $\langle S_z \rangle^{eff}$ of 11.44 (Ho), 6.08 (Er), 4.71 (Tm) and 1.37 (Yb).

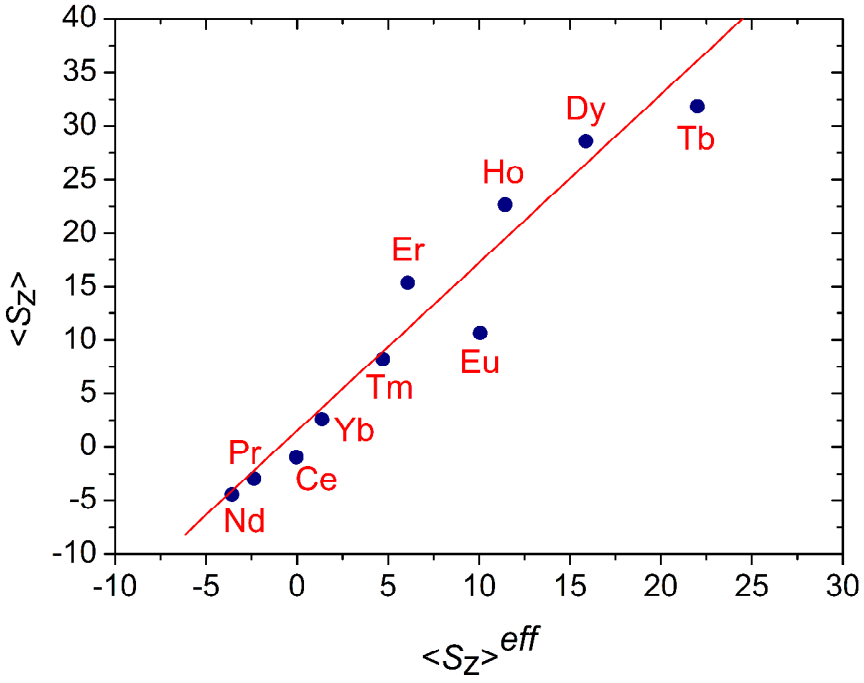

Figure S14. Plots of the $\langle S_z \rangle^{eff}$ values obtained for $[LnL^1]^{3+}$ complexes versus the $\langle S_z \rangle$ theoretical values. The solid line corresponds to the linear fit of the data ($R^2 > 0.98$).

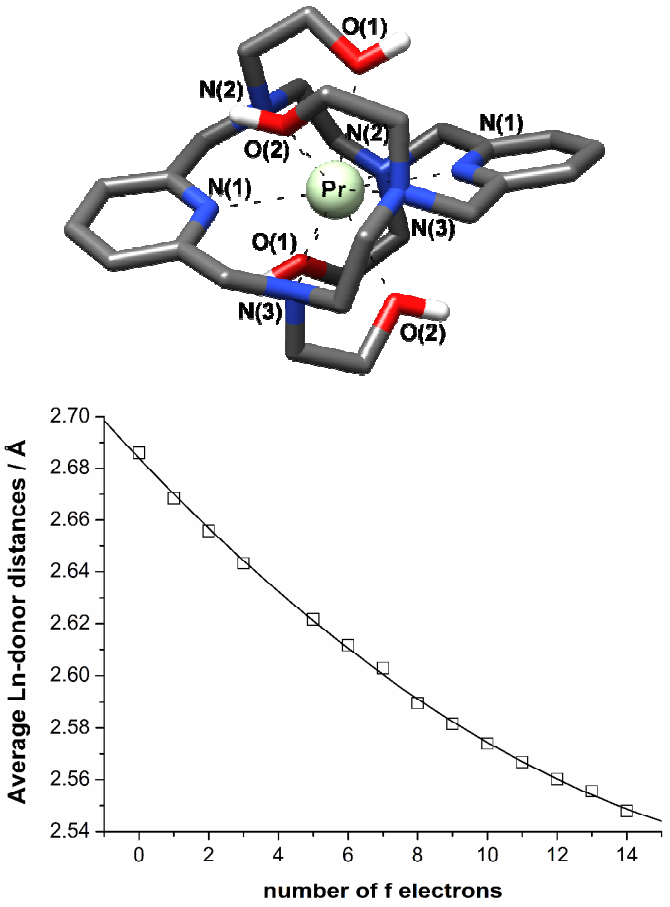

Figure S15. Variation of the average calculated bond distances of the metal coordination environments for $[LnL^1]^{3+}$ complexes at the TPSSh/LCRECP/6-31G(d,p) level. The solid line represents quadratic fits of the data to $y = a + bx + cx^2$ with $R^2 > 0.999$.

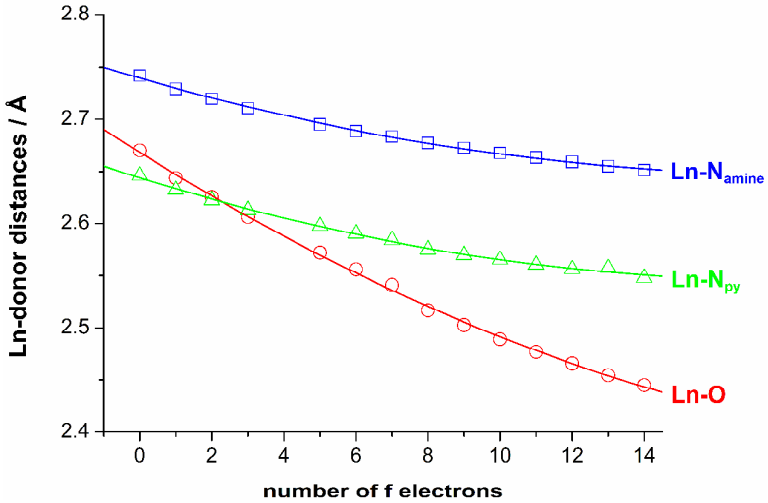

Figure S16. Variation of the calculated bond distances of the metal coordination environments for $[LnL^1]^{3+}$ complexes at the TPSSh/LCRECP/6-31G(d,p) level. The solid lines represent quadratic fits of the data to $y = a + bx + cx^2$ with $R^2 > 0.99$.

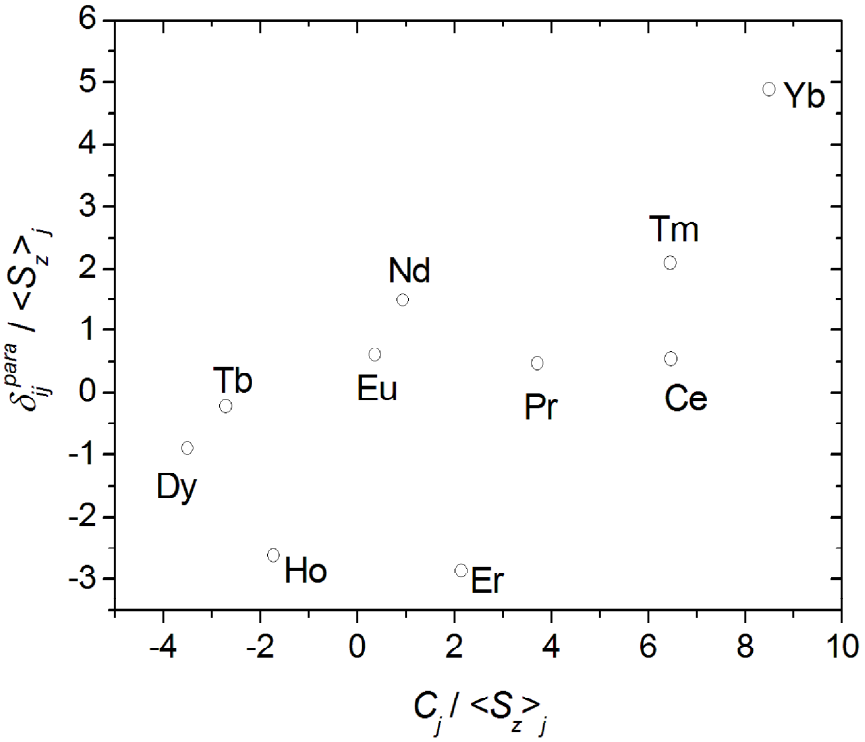

Figure S17. Plot according to Realley's method for protons H1 in $[LnL^1]^{3+}$ complexes.

Table S1. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[CeL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-0.53	0.13	0.00	-0.53
H2	-0.83	-0.66	0.00	-0.83
H3ax	-10.29	-11.14	0.01	-10.30
H3eq	-5.00	-5.44	-0.04	-4.96
H4ax	-13.73	-13.88	0.00	-13.73
H4eq	-10.44	-10.61	-0.07	-10.37
H5ax	11.97	10.96	0.00	11.97
H5eq	-0.05	-0.44	-0.03	-0.02
H6ax	0.91	2.05	-0.02	0.93
H6eq	12.03	11.42	0.01	12.02

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S2. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[PrL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-1.38	-0.81	-0.27	-1.11
H2	-2.77	-2.28	-0.16	-2.61
H3ax	-19.00	-20.14	0.54	-19.54
H3eq	-11.97	-12.93	-2.75	-9.22
H4ax	-23.40	-23.36	0.06	-23.46
H4eq	-22.42	-22.53	-4.41	-18.01
H5ax	21.29	20.37	0.14	21.15
H5eq	-2.80	-2.17	-2.13	-0.67
H6ax	3.03	3.48	-1.59	4.62
H6eq	23.76	23.02	0.68	23.08

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S3. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[NdL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-6.65	-6.24	-0.41	-6.24
H2	-8.68	-7.88	-0.24	-8.44
H3ax	-11.26	-11.96	0.81	-12.07
H3eq	-11.54	-12.41	-4.15	-7.39
H4ax	1.51	1.66	0.09	1.42
H4eq	-8.53	-8.43	-6.65	-1.88
H5ax	10.73	10.44	0.21	10.52
H5eq	0.77	1.07	-3.21	3.98
H6ax	8.37	8.71	-2.40	10.77
H6eq	22.66	22.14	1.03	21.63

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S4. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[EuL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	6.52	6.97	1.15	5.37
H2	9.67	8.66	0.68	8.99
H3ax	15.88	15.27	-2.29	18.17
H3eq	22.06	22.10	11.68	10.38
H4ax	4.42	4.17	-0.25	4.67
H4eq	24.75	24.90	18.70	6.05
H5ax	-15.57	-16.30	-0.60	-14.97
H5eq	6.14	4.43	9.02	-2.88
H6ax	-6.44	-5.70	6.75	-13.19
H6eq	-29.72	-29.98	-2.90	-26.82

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S5. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[TbL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-6.98	-9.45	2.52	-9.50
H2	-18.02	-22.87	1.49	-19.51
H3ax	-144.47	-153.58	-5.01	-139.46
H3eq	-43.47	-47.17	25.55	-69.02
H4ax	-145.78	-146.72	-0.55	-145.23
H4eq	-74.75	-74.60	40.92	-115.67
H5ax	150.14	145.92	-1.30	151.44
H5eq	27.95	29.31	19.74	8.21
H6ax	65.15	67.16	14.76	50.39
H6eq	182.35	174.65	-6.34	188.69

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S6. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[DyL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-25.51	-27.64	1.81	-27.32
H2	-41.57	-44.81	1.07	-42.64
H3ax	-162.84	-171.43	-3.61	-159.23
H3eq	-65.37	-69.00	18.43	-83.80
H4ax	-120.41	-119.64	-0.40	-120.01
H4eq	-73.09	-74.00	29.51	-102.60
H5ax	164.23	162.07	-0.94	165.17
H5eq	36.81	39.45	14.24	22.57
H6ax	93.32	93.90	10.65	82.67
H6eq	232.50	225.14	-4.57	237.07

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S7. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[HoL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-59.33	-60.86	1.31	-60.64
H2	-75.97	-77.94	0.77	-76.74
H3ax	-96.41	-100.86	-2.60	-93.81
H3eq	-50.05	-54.04	13.28	-63.33
H4ax	56.77	59.19	-0.29	57.06
H4eq	35.94	37.23	21.27	14.67
H5ax	82.26	89.32	-0.68	82.94
H5eq	64.65	66.18	10.26	54.38
H6ax	122.97	120.78	7.68	115.29
H6eq	201.64	193.83	-3.30	204.94

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S8. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[ErL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	-44.03	-43.75	0.69	-44.72
H2	-50.25	-49.83	0.41	-50.66
H3ax	10.28	13.14	-1.38	11.66
H3eq	1.13	-2.24	7.06	-5.93
H4ax	140.97	145.48	-0.15	141.12
H4eq	99.39	100.20	11.30	88.09
H5ax	-29.34	-20.23	-0.36	-28.98
H5eq	47.23	46.30	5.45	41.78
H6ax	48.75	49.58	4.08	44.67
H6eq	68.14	58.18	-1.75	69.89

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S9. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[TmL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	17.22	20.09	0.54	16.68
H2	26.14	29.31	0.32	25.82
H3ax	87.27	89.57	-1.07	88.34
H3eq	59.59	53.65	5.47	54.12
H4ax	56.09	54.17	-0.12	56.21
H4eq	52.67	58.31	8.76	43.91
H5ax	-89.40	-89.43	-0.28	-89.12
H5eq	-11.83	-13.61	4.22	-16.05
H6ax	-45.13	-47.73	3.16	-48.29
H6eq	-135.29	-132.32	-1.36	-133.93

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S10. Comparison of experimental and calculated δ_{ij}^{para} values, contact (δ_{ij}^{con}) and pseudocontact (δ_{ij}^{pscon}) contributions obtained for $[YbL^1]^{3+}$.

	δ_{ij}^{para} (exp.)	δ_{ij}^{para} (cald.)[a]	δ_{ij}^{con} [a]	δ_{ij}^{pscon} [a]
H1	12.66	13.24	0.16	12.50
H2	16.92	18.00	0.093	16.83
H3ax	37.72	39.56	-0.31	38.03
H3eq	24.40	24.29	1.59	22.81
H4ax	11.62	11.03	-0.03	11.65
H4eq	16.34	16.70	2.55	13.79
H5ax	-38.70	-39.32	-0.08	-38.62
H5eq	-11.48	-10.97	1.23	-12.71
H6ax	-27.50	-27.94	0.92	-28.42
H6eq	-66.48	-64.57	-0.39	-66.08

[a] Calculated values were obtained using Eq. (1), Eq. (2) and the geometry of the complex optimized in solution at the TPSSh/LCRECP/6-31G(d,p).

Table S11. Results of the quadratic fits ($y = a + bx + cx^2$) for the Ln-donor distances calculated for different series of complexes.[a]

	$[Ln(H_2O)_8]^{3+}$	$[LnL^1]^{3+}$
a(σ)	2.556(2)	2.684(1)
10^2 b(σ)	-2.04(6)	-1.42(3)
10^4 c(σ)	3.92	3.23(22)
10^3 b* = b/a	-7.997	-5.291
10^4 c* = c/a	1.532	1.203
10^2 c/b	-1.92	-2.27
R^2	0.9993	0.9991

[a] Bond distances for the $[Ln(H_2O)_8]^{3+}$ complexes taken from ref. [1].

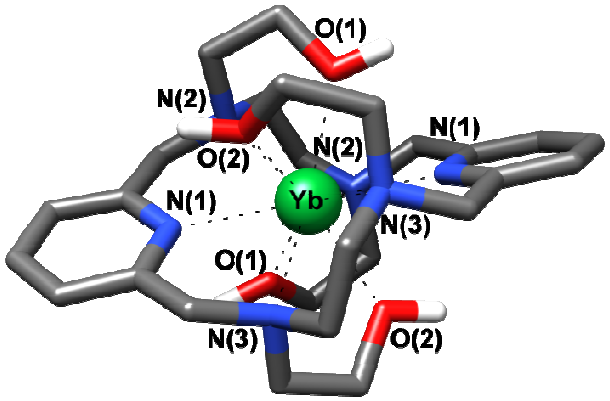

Table S12. Average bond distances (Å) of the metal coordination environments in $[LnL^1]^{3+}$ complexes obtained from DFT calculations (aqueous solution, TPSSh/LCRECP/6-31G(d,p) level).

	Ln-N_{py}	**Ln-N_{amine}**	**Ln-O**
$[LaL^1]^{3+}$	2.646	2.742	2.670
$[CeL^1]^{3+}$	2.632	2.729	2.644
$[PrL^1]^{3+}$	2.622	2.720	2.625
$[NdL^1]^{3+}$	2.613	2.711	2.606
$[SmL^1]^{3+}$	2.598	2.695	2.572
$[EuL^1]^{3+}$	2.590	2.689	2.556
$[GdL^1]^{3+}$	2.584	2.683	2.541
$[TbL^1]^{3+}$	2.575	2.677	2.517
$[DyL^1]^{3+}$	2.570	2.672	2.503
$[HoL^1]^{3+}$	2.565	2.668	2.489
$[ErL^1]^{3+}$	2.560	2.663	2.477
$[TmL^1]^{3+}$	2.556	2.659	2.466
$[YbL^1]^{3+}$	2.557	2.655	2.454
$[LuL^1]^{3+}$	2.548	2.651	2.445

Table S13. $[LaL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	57	0.000121	-0.000459	0.000679
2	7	2.645917	0.000660	-0.000736
3	7	1.198063	2.287893	-0.920801
4	7	-1.199108	2.287126	0.921212
5	7	-2.645909	-0.000026	0.000690
6	7	-1.198824	-2.287739	-0.920467
7	7	1.199829	-2.287194	0.920596
8	8	-0.825803	1.171909	-2.252208
9	8	0.825353	1.171286	2.253441
10	8	0.823995	-1.172217	-2.252421
11	8	-0.823713	-1.171699	2.253997
12	6	3.323459	-1.158246	0.168843
13	6	4.718868	-1.188834	0.191275
14	1	5.240454	-2.126382	0.346911
15	6	5.421062	0.001030	-0.002762
16	1	6.505794	0.001183	-0.003556
17	6	4.718255	1.190716	-0.195757
18	1	5.239360	2.128406	-0.352151
19	6	3.322903	1.159741	-0.171295
20	6	2.517526	2.444650	-0.253730
21	1	2.331200	2.790414	0.767780
22	1	3.115468	3.218017	-0.754181
23	6	0.341717	3.489721	-0.680044
24	1	-0.410712	3.525469	-1.466965
25	1	0.938405	4.407405	-0.770358
26	6	-0.342953	3.489190	0.681581
27	1	0.409435	3.524354	1.468583
28	1	-0.939649	4.406806	0.772597
29	6	-2.518531	2.444052	0.254231
30	1	-2.332333	2.791089	-0.766866
31	1	-3.116814	3.216575	0.755591
32	6	-3.323376	1.158885	0.170193
33	6	-4.718801	1.189646	0.192234
34	1	-5.240316	2.127254	0.347755
35	6	-5.421087	-0.000106	-0.002023
36	1	-6.505819	-0.000128	-0.003099
37	6	-4.718355	-1.189881	-0.194842
38	1	-5.239539	-2.127505	-0.351364
39	6	-3.323017	-1.159062	-0.170061
40	6	-2.517874	-2.444138	-0.252459
41	1	-2.330900	-2.789601	0.769032
42	1	-3.116232	-3.217566	-0.752298
43	6	-0.342252	-3.489518	-0.680192
44	1	0.409636	-3.525237	-1.467623
45	1	-0.938951	-4.407235	-0.770051
46	6	0.343430	-3.489190	0.680945
47	1	-0.408367	-3.524714	1.468472
48	1	0.940228	-4.406816	0.771158
49	6	2.518733	-2.443536	0.252397
50	1	2.331633	-2.789581	-0.768878
51	1	3.117469	-3.216456	0.752578
52	6	1.404080	2.094534	-2.381893
53	1	2.056230	1.226965	-2.503603

54	1	1.923424	2.956338	-2.823959
55	6	0.083431	1.887994	-3.126322
56	6	-1.405342	2.092274	2.382131
57	1	-2.056346	1.223729	2.502799
58	1	-1.925877	2.953076	2.824730
59	6	-0.084819	1.886781	3.126981
60	6	-1.405800	-2.094505	-2.381466
61	1	-2.057653	-1.226692	-2.502851
62	1	-1.925611	-2.956285	-2.823006
63	6	-0.085571	-1.888188	-3.126622
64	6	1.406941	-2.093018	2.381464
65	1	2.058241	-1.224696	2.502182
66	1	1.927470	-2.954145	2.823439
67	6	0.086820	-1.887442	3.127062
68	1	-0.263084	1.311423	4.039081
69	1	0.373765	2.839394	3.404212
70	1	0.265528	-1.312186	4.039133
71	1	-0.371750	-2.840022	3.404382
72	1	-0.263857	-1.312548	-4.038486
73	1	0.373797	-2.840426	-3.403810
74	1	0.261537	1.312676	-4.038478
75	1	-0.375957	2.840267	-3.403415
76	1	1.685055	-1.102242	-2.691914
77	1	-1.688099	1.105872	-2.689855
78	1	-1.686158	-1.107598	2.691648
79	1	1.687892	1.106939	2.690854

E(RTPSSh) = -1676.9945079 Hartree
Zero-point correction = 0.689677 Hartree/particle
Sum of electronic and thermal Energies = -1676.269564 Hartree
Sum of electronic and thermal Enthalpies = -1676.268620 Hartree
Sum of electronic and thermal Free Energies = -1676.365862 Hartree

Table S14. $[CeL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	58	-0.000072	0.000083	-0.000101
2	7	-2.632216	-0.000141	-0.000496
3	7	-1.179810	-2.275086	-0.938301
4	7	1.180016	-2.274669	0.938638
5	7	2.632228	0.000106	0.000755
6	7	1.180267	2.275137	-0.937670
7	7	-1.180348	2.274709	0.938231
8	8	0.857342	-1.144304	-2.223707
9	8	-0.857295	-1.144105	2.223862
10	8	-0.856396	1.144932	-2.223819
11	8	0.856147	1.143605	2.224535
12	6	-3.311197	1.154609	0.191949
13	6	-4.706565	1.184795	0.217017
14	1	-5.227306	2.119393	0.392021
15	6	-5.409574	-0.000154	-0.001211
16	1	-6.494289	-0.000152	-0.001503
17	6	-4.706447	-1.185106	-0.219055
18	1	-5.227088	-2.119712	-0.394311

19	6	-3.311093	-1.154899	-0.193255
20	6	-2.509460	-2.439676	-0.294504
21	1	-2.340061	-2.808981	0.721606
22	1	-3.102827	-3.200290	-0.819278
23	6	-0.329091	-3.478456	-0.686340
24	1	0.437613	-3.513662	-1.459427
25	1	-0.925170	-4.395125	-0.789641
26	6	0.329280	-3.478149	0.687204
27	1	-0.437420	-3.512981	1.460311
28	1	0.925352	-4.394778	0.790914
29	6	2.509555	-2.439464	0.294698
30	1	2.340059	-2.809081	-0.721287
31	1	3.103029	-3.199872	0.819662
32	6	3.311144	-1.154715	0.192837
33	6	4.706535	-1.185083	0.217367
34	1	5.227217	-2.119765	0.392098
35	6	5.409610	-0.000229	-0.001068
36	1	6.494325	-0.000372	-0.001810
37	6	4.706536	1.184834	-0.218565
38	1	5.227214	2.119385	-0.394002
39	6	3.311205	1.154798	-0.192207
40	6	2.509594	2.439591	-0.293145
41	1	2.339646	2.808344	0.723075
42	1	3.103144	3.200498	-0.817282
43	6	0.329442	3.478515	-0.686091
44	1	-0.436890	3.513696	-1.459554
45	1	0.925586	4.395169	-0.789121
46	6	-0.329543	3.478198	0.687156
47	1	0.436803	3.513040	1.460616
48	1	-0.925672	4.394817	0.790613
49	6	-2.509641	2.439382	0.293679
50	1	-2.339687	2.808667	-0.722348
51	1	-3.103295	3.199949	0.818201
52	6	-1.360299	-2.081407	-2.402949
53	1	-2.011984	-1.216226	-2.537975
54	1	-1.866316	-2.945698	-2.855183
55	6	-0.025938	-1.866840	-3.119239
56	6	1.360713	-2.080631	2.403187
57	1	2.012437	-1.215443	2.537894
58	1	1.866727	-2.944866	2.855535
59	6	0.026429	-1.865779	3.119651
60	6	1.361478	2.081643	-2.402228
61	1	2.013284	1.216522	-2.537041
62	1	1.867636	2.946039	-2.854101
63	6	0.027416	1.867045	-3.119128
64	6	-1.361697	2.080666	2.402705
65	1	-2.013448	1.215459	2.537126
66	1	-1.867904	2.944903	2.854834
67	6	-0.027755	1.865767	3.119753
68	1	0.187438	-1.291088	4.035235
69	1	-0.446019	-2.814414	3.386552
70	1	-0.189278	1.291376	4.035437
71	1	0.444812	2.814369	3.386561
72	1	0.188656	1.292785	-4.034941
73	1	-0.445066	2.815775	-3.385678
74	1	-0.186786	-1.292889	-4.035313
75	1	0.446814	-2.815576	-3.385266
76	1	-1.735506	1.092453	-2.628648
77	1	1.736754	-1.092245	-2.627925
78	1	1.735973	1.093604	2.628104

79	1	-1.737485	-1.094799	2.626726

E(RTPSSh) = -1677.6463873 Hartree
Zero-point correction = 0.688452 Hartree/particle
Sum of electronic and thermal Energies = -1676.922175 Hartree
Sum of electronic and thermal Enthalpies = -1676.921230 Hartree
Sum of electronic and thermal Free Energies = -1677.020366 Hartree

Table S15. $[PrL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	59	-0.000142	0.000199	0.000294
2	7	-2.622340	-0.000330	-0.000777
3	7	-1.168352	-2.266282	-0.946227
4	7	1.169097	-2.265898	0.946493
5	7	2.622284	0.000207	0.000643
6	7	1.168875	2.266252	-0.945831
7	7	-1.169608	2.266116	0.945743
8	8	0.873443	-1.126152	-2.204418
9	8	-0.872715	-1.125751	2.205465
10	8	-0.871632	1.125157	-2.205652
11	8	0.871482	1.126009	2.205808
12	6	-3.302934	1.151868	0.202083
13	6	-4.698259	1.181683	0.228010
14	1	-5.218496	2.114899	0.411666
15	6	-5.401603	-0.000813	-0.001060
16	1	-6.486303	-0.001001	-0.001180
17	6	-4.697802	-1.183060	-0.229960
18	1	-5.217677	-2.116461	-0.413703
19	6	-3.302482	-1.152764	-0.203722
20	6	-2.502695	-2.436863	-0.314889
21	1	-2.342061	-2.819185	0.697782
22	1	-3.092911	-3.190667	-0.852797
23	6	-0.320597	-3.470593	-0.689868
24	1	0.454525	-3.503680	-1.454663
25	1	-0.915954	-4.386600	-0.802345
26	6	0.321579	-3.470419	0.690330
27	1	-0.453589	-3.503556	1.455068
28	1	0.917073	-4.386321	0.802973
29	6	2.503427	-2.436346	0.315174
30	1	2.342903	-2.819353	-0.697249
31	1	3.093930	-3.189639	0.853492
32	6	3.302795	-1.152040	0.203277
33	6	4.698148	-1.182072	0.228631
34	1	5.218299	-2.115382	0.412052
35	6	5.401583	0.000295	-0.000705
36	1	6.486284	0.000322	-0.001260
37	6	4.697850	1.182654	-0.229333
38	1	5.217780	2.115983	-0.413281
39	6	3.302552	1.152537	-0.202615
40	6	2.502867	2.436703	-0.313731
41	1	2.341699	2.818764	0.698952
42	1	3.093362	3.190627	-0.851165
43	6	0.321004	3.470590	-0.690040

44	1	-0.453685	3.503655	-1.455277
45	1	0.916406	4.386602	-0.802249
46	6	-0.321985	3.470618	0.689788
47	1	0.452714	3.503945	1.454992
48	1	-0.917600	4.386504	0.801882
49	6	-2.503605	2.436233	0.313549
50	1	-2.342462	2.818487	-0.699064
51	1	-3.094388	3.189894	0.851035
52	6	-1.336337	-2.073289	-2.412429
53	1	-1.991544	-1.212402	-2.554290
54	1	-1.831667	-2.941174	-2.869456
55	6	0.004709	-1.849912	-3.113163
56	6	1.337224	-2.072459	2.412671
57	1	1.991844	-1.211066	2.554173
58	1	1.833226	-2.939899	2.869820
59	6	-0.003740	-1.849866	3.113659
60	6	1.337785	2.073035	-2.411935
61	1	1.992671	1.211818	-2.553231
62	1	1.833728	2.940695	-2.868720
63	6	-0.002806	1.850058	-3.113455
64	6	-1.338469	2.073042	2.411875
65	1	-1.993312	1.211798	2.553270
66	1	-1.834539	2.940674	2.868574
67	6	0.002159	1.850346	3.113523
68	1	0.148286	-1.274289	4.030127
69	1	-0.484344	-2.795521	3.376338
70	1	-0.150374	1.274856	4.029961
71	1	0.482766	2.795954	3.376351
72	1	0.149778	1.274786	-4.030016
73	1	-0.483898	2.795510	-3.375973
74	1	-0.147387	-1.273751	-4.029250
75	1	0.485581	-2.795269	-3.376413
76	1	-1.761395	1.086080	-2.588104
77	1	1.763822	-1.088735	-2.585602
78	1	1.761420	1.088062	2.587966
79	1	-1.762660	-1.087271	2.587557

E(RTPSSh) = -1678.2804078 Hartree
Zero-point correction = 0.689001 Hartree/particle
Sum of electronic and thermal Energies = -1677.555863 Hartree
Sum of electronic and thermal Enthalpies = -1677.554919 Hartree
Sum of electronic and thermal Free Energies = -1677.653316 Hartree

Table S16. $[NdL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	60	-0.000028	0.000041	0.000072
2	7	-2.613052	-0.000031	-0.000312
3	7	-1.159547	-2.257575	-0.951783
4	7	1.159629	-2.257332	0.952225
5	7	2.613005	0.000060	0.000343
6	7	1.159755	2.257396	-0.951930
7	7	-1.159904	2.257587	0.951542
8	8	0.883493	-1.109357	-2.186571

9	8	-0.883275	-1.108776	2.187016
10	8	-0.882635	1.108430	-2.187436
11	8	0.882753	1.109262	2.187035
12	6	-3.294986	1.150277	0.209507
13	6	-4.690275	1.180325	0.235736
14	1	-5.209685	2.112860	0.425102
15	6	-5.394330	-0.000129	-0.000517
16	1	-6.479016	-0.000169	-0.000595
17	6	-4.690155	-1.180531	-0.236667
18	1	-5.209472	-2.113104	-0.426106
19	6	-3.294869	-1.150388	-0.210231
20	6	-2.496888	-2.433754	-0.329483
21	1	-2.342381	-2.826531	0.680091
22	1	-3.084614	-3.182106	-0.877540
23	6	-0.313975	-3.462489	-0.692476
24	1	0.468370	-3.493065	-1.450060
25	1	-0.908304	-4.378083	-0.813189
26	6	0.314032	-3.462296	0.693264
27	1	-0.468320	-3.492608	1.450856
28	1	0.908327	-4.377874	0.814255
29	6	2.496936	-2.433618	0.329882
30	1	2.342378	-2.826604	-0.679600
31	1	3.084710	-3.181836	0.878072
32	6	3.294872	-1.150251	0.210321
33	6	4.690165	-1.180360	0.236562
34	1	5.209530	-2.112896	0.426048
35	6	5.394278	0.000026	0.000161
36	1	6.478965	0.000011	0.000086
37	6	4.690163	1.180436	-0.236151
38	1	5.209527	2.112956	-0.425719
39	6	3.294881	1.150358	-0.209732
40	6	2.496907	2.433704	-0.329241
41	1	2.342083	2.826517	0.680268
42	1	3.084751	3.182042	-0.877189
43	6	0.314040	3.462319	-0.693167
44	1	-0.468139	3.492583	-1.450941
45	1	0.908307	4.377932	-0.814037
46	6	-0.314293	3.462512	0.692428
47	1	0.467869	3.493105	1.450202
48	1	-0.908658	4.378101	0.812992
49	6	-2.497097	2.433688	0.328890
50	1	-2.342355	2.826431	-0.680661
51	1	-3.084990	3.182037	0.876773
52	6	-1.318959	-2.065810	-2.419026
53	1	-1.980035	-1.210658	-2.566198
54	1	-1.803294	-2.938152	-2.879233
55	6	0.026669	-1.831890	-3.107563
56	6	1.319164	-2.065254	2.419412
57	1	1.980232	-1.210050	2.566346
58	1	1.803572	-2.937484	2.879753
59	6	-0.026409	-1.831252	3.108023
60	6	1.319692	2.065325	-2.419074
61	1	1.980836	1.210148	-2.565823
62	1	1.804187	2.937575	-2.879288
63	6	-0.025660	1.831244	-3.108063
64	6	-1.319715	2.065823	2.418743
65	1	-1.980772	1.210620	2.565730
66	1	-1.804246	2.938131	2.878807
67	6	0.025717	1.832001	3.107675
68	1	0.119449	-1.250316	4.022046

69	1	-0.514590	-2.772613	3.371967
70	1	-0.120328	1.251324	4.021833
71	1	0.513858	2.773428	3.371461
72	1	0.120542	1.250523	-4.022171
73	1	-0.513924	2.772577	-3.371955
74	1	-0.119113	-1.251047	-4.021657
75	1	0.514844	-2.773289	-3.371389
76	1	-1.779785	1.075764	-2.552911
77	1	1.780659	-1.076418	-2.551989
78	1	1.779839	1.076409	2.552656
79	1	-1.780474	-1.075970	2.552363

E(RTPSSh) = -1678.9023195 Hartree
Zero-point correction = 0.689233 Hartree/particle
Sum of electronic and thermal Energies = -1678.177630 Hartree
Sum of electronic and thermal Enthalpies = -1678.176686 Hartree
Sum of electronic and thermal Free Energies = -1678.274834 Hartree

Table S17. $[SmL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	62	0.000036	0.000039	0.000006
2	7	2.597590	0.000050	0.000393
3	7	1.145945	-2.243952	0.956442
4	7	-1.145820	-2.243594	-0.957234
5	7	-2.597524	-0.000018	-0.000385
6	7	-1.146171	2.243558	0.956983
7	7	1.146145	2.244043	-0.956083
8	8	-0.895356	-1.083495	2.154170
9	8	0.895174	-1.082300	-2.154819
10	8	0.894386	1.082050	2.155386
11	8	-0.894640	1.083320	-2.154555
12	6	3.282307	1.147745	-0.216380
13	6	4.677492	1.178074	-0.242730
14	1	5.195584	2.110186	-0.437705
15	6	5.382560	0.000003	0.000315
16	1	6.467223	-0.000017	0.000278
17	6	4.677466	-1.178037	0.243400
18	1	5.195537	-2.110170	0.438334
19	6	3.282273	-1.147663	0.217126
20	6	2.486916	-2.429503	0.346763
21	1	2.340970	-2.836677	-0.658333
22	1	3.070494	-3.170355	0.909126
23	6	0.304344	-3.450707	0.695554
24	1	-0.487563	-3.477607	1.443328
25	1	0.897941	-4.364998	0.828311
26	6	-0.304116	-3.450391	-0.696921
27	1	0.487812	-3.476819	-1.444695
28	1	-0.897607	-4.364682	-0.830146
29	6	-2.486744	-2.429436	-0.347537
30	1	-2.340703	-2.836842	0.657447
31	1	-3.070287	-3.170180	-0.910078
32	6	-3.282170	-1.147673	-0.217556
33	6	-4.677357	-1.178052	-0.244010

34	1	-5.195398	-2.110128	-0.439290
35	6	-5.382490	-0.000085	-0.000670
36	1	-6.467152	-0.000109	-0.000785
37	6	-4.677463	1.177915	0.242828
38	1	-5.195587	2.109965	0.438013
39	6	-3.282272	1.147600	0.216668
40	6	-2.486920	2.429386	0.346882
41	1	-2.340598	2.836823	-0.658048
42	1	-3.070645	3.170100	0.909275
43	6	-0.304400	3.450368	0.696940
44	1	0.487330	3.476764	1.444924
45	1	-0.897918	4.364659	0.830050
46	6	0.304430	3.450753	-0.695378
47	1	-0.487276	3.477645	-1.443368
48	1	0.898019	4.365076	-0.827946
49	6	2.486944	2.429579	-0.346007
50	1	2.340696	2.836589	0.659111
51	1	3.070636	3.170545	-0.908101
52	6	1.294231	-2.054208	2.424868
53	1	1.964813	-1.208222	2.579893
54	1	1.761870	-2.933322	2.889268
55	6	-0.057772	-1.804060	3.094591
56	6	-1.294265	-2.053252	-2.425567
57	1	-1.964881	-1.207210	-2.580166
58	1	-1.761951	-2.932177	-2.890277
59	6	0.057650	-1.802815	-3.095333
60	6	-1.295087	2.053167	2.425263
61	1	-1.965703	1.207078	2.579608
62	1	-1.762978	2.932052	2.889844
63	6	0.056597	1.802780	3.095494
64	6	1.294869	2.054338	-2.424471
65	1	1.965491	1.208347	-2.579315
66	1	1.762657	2.933457	-2.888710
67	6	-0.056917	1.804200	-3.094610
68	1	-0.078848	-1.215193	-4.006386
69	1	0.557875	-2.737634	-3.359800
70	1	0.079759	1.216945	-4.005873
71	1	-0.557076	2.739131	-3.358806
72	1	-0.080235	1.215328	4.006610
73	1	0.556774	2.737621	3.359974
74	1	0.078590	-1.216592	4.005761
75	1	-0.557885	-2.738996	3.358860
76	1	1.798837	1.045214	2.502082
77	1	-1.799826	-1.046418	2.500796
78	1	-1.799015	1.046153	-2.501420
79	1	1.799667	-1.045170	-2.501380

E(RTPSSh) = -1680.1231015 Hartree
Zero-point correction = 0.689504 Hartree/particle
Sum of electronic and thermal Energies = -1679.398203 Hartree
Sum of electronic and thermal Enthalpies = -1679.397258 Hartree
Sum of electronic and thermal Free Energies = -1679.495193 Hartree

Table S18. $[EuL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.000040	-0.000164	-0.000105
2	7	-2.590305	0.000071	0.000509
3	7	-1.139742	2.238709	0.958259
4	7	1.139940	2.238546	-0.958485
5	7	2.590321	0.000017	-0.000309
6	7	1.139985	-2.238564	0.958239
7	7	-1.140181	-2.238711	-0.957908
8	8	0.900072	1.072698	2.138207
9	8	-0.899814	1.072168	-2.138591
10	8	-0.899127	-1.071581	2.139072
11	8	0.899262	-1.072844	-2.138704
12	6	-3.276370	-1.146462	-0.219175
13	6	-4.671520	-1.176783	-0.245714
14	1	-5.189067	-2.108694	-0.443067
15	6	-5.376988	0.000317	0.000034
16	1	-6.461636	0.000411	-0.000142
17	6	-4.671395	1.177283	0.245995
18	1	-5.188838	2.109297	0.443138
19	6	-3.276227	1.146719	0.219909
20	6	-2.482122	2.427966	0.353758
21	1	-2.339667	2.840959	-0.649437
22	1	-3.064105	3.165563	0.921962
23	6	-0.300263	3.446605	0.697287
24	1	0.495196	3.472380	1.441317
25	1	-0.894063	4.359998	0.834835
26	6	0.300582	3.446542	-0.697575
27	1	-0.494913	3.472369	-1.441559
28	1	0.894446	4.359881	-0.835196
29	6	2.482377	2.427834	-0.354149
30	1	2.340043	2.841213	0.648902
31	1	3.064387	3.165182	-0.922647
32	6	3.276355	1.146539	-0.219984
33	6	4.671525	1.176981	-0.246123
34	1	5.189032	2.108927	-0.443415
35	6	5.377021	-0.000016	-0.000041
36	1	6.461669	-0.000026	0.000083
37	6	4.671445	-1.177010	0.245892
38	1	5.188906	-2.108958	0.443296
39	6	3.276293	-1.146545	0.219477
40	6	2.482244	-2.427809	0.353467
41	1	2.339583	-2.840842	-0.649681
42	1	3.064340	-3.165369	0.921602
43	6	0.300540	-3.446558	0.697583
44	1	-0.494741	-3.472367	1.441794
45	1	0.894422	-4.359909	0.835045
46	6	-0.300705	-3.446668	-0.697112
47	1	0.494553	-3.472534	-1.441354
48	1	-0.894612	-4.360019	-0.834442
49	6	-2.482393	-2.427793	-0.352933
50	1	-2.339625	-2.840595	0.650293
51	1	-3.064583	-3.165469	-0.920819
52	6	-1.283235	2.049857	2.427051
53	1	-1.958327	1.208245	2.585639

54	1	-1.743075	2.932007	2.893403
55	6	0.071482	1.791815	3.088030
56	6	1.283324	2.049307	-2.427279
57	1	1.957940	1.207273	-2.585661
58	1	1.743605	2.931103	-2.893863
59	6	-0.071485	1.791856	-3.088144
60	6	1.283833	-2.049244	2.427000
61	1	1.958383	-1.207113	2.585115
62	1	1.744306	-2.930998	2.893465
63	6	-0.070757	-1.791808	3.088253
64	6	-1.284111	-2.049861	-2.426684
65	1	-1.958963	-1.208015	-2.585072
66	1	-1.744382	-2.931877	-2.892852
67	6	0.070469	-1.792311	-3.088056
68	1	0.060718	1.201616	-3.998028
69	1	-0.577154	2.723788	-3.352288
70	1	-0.062086	-1.201850	-3.997742
71	1	0.575987	-2.724208	-3.352604
72	1	0.061743	-1.201891	3.998306
73	1	-0.576598	-2.723705	3.352181
74	1	-0.061011	1.200886	3.997420
75	1	0.577168	2.723503	3.352970
76	1	-1.805372	-1.026381	2.479923
77	1	1.806714	1.029089	2.478215
78	1	1.805485	-1.027979	-2.479664
79	1	-1.806098	1.026930	-2.479339

E(RTPSSh) = -1680.7190885 Hartree
Zero-point correction = 0.689700 Hartree/particle
Sum of electronic and thermal Energies = -1679.994030 Hartree
Sum of electronic and thermal Enthalpies = -1679.993085 Hartree
Sum of electronic and thermal Free Energies = -1680.091015 Hartree

Table S19. $[GdL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	0.000091	-0.000144	0.000272
2	7	2.584034	0.000255	-0.000365
3	7	1.134203	2.234278	-0.960473
4	7	-1.134788	2.234177	0.960274
5	7	-2.584087	-0.000156	0.000113
6	7	-1.134342	-2.234346	-0.960156
7	7	1.134855	-2.234104	0.960276
8	8	-0.904693	1.062267	-2.123080
9	8	0.904162	1.062268	2.124120
10	8	0.904060	-1.061542	-2.124064
11	8	-0.903875	-1.062371	2.124138
12	6	3.271246	-1.145149	0.222415
13	6	4.666396	-1.175510	0.248669
14	1	5.183483	-2.107139	0.448553
15	6	5.372197	0.000515	-0.000554
16	1	6.456833	0.000616	-0.000642
17	6	4.666140	1.176408	-0.249659
18	1	5.183025	2.108135	-0.449605

19	6	3.270997	1.145788	-0.223189
20	6	2.478094	2.426618	-0.361196
21	1	2.339218	2.845282	0.640148
22	1	3.058690	3.160905	-0.935013
23	6	0.296499	3.442981	-0.698773
24	1	-0.502165	3.467965	-1.439396
25	1	0.890355	4.355668	-0.840431
26	6	-0.297426	3.443071	0.698273
27	1	0.501306	3.468517	1.438788
28	1	-0.891506	4.355643	0.839721
29	6	-2.478736	2.426238	0.361074
30	1	-2.340024	2.845254	-0.640144
31	1	-3.059513	3.160206	0.935116
32	6	-3.271313	1.145239	0.222749
33	6	-4.666479	1.175659	0.248729
34	1	-5.183553	2.107330	0.448450
35	6	-5.372273	-0.000342	-0.000571
36	1	-6.456909	-0.000414	-0.000858
37	6	-4.666193	-1.176264	-0.249517
38	1	-5.183063	-2.107989	-0.449516
39	6	-3.271059	-1.145665	-0.222841
40	6	-2.478203	-2.426527	-0.360774
41	1	-2.339277	-2.845123	0.640593
42	1	-3.058851	-3.160837	-0.934507
43	6	-0.296800	-3.443139	-0.698271
44	1	0.501814	-3.468482	-1.438918
45	1	-0.890786	-4.355783	-0.839646
46	6	0.297336	-3.442994	0.698690
47	1	-0.501258	-3.468160	1.439367
48	1	0.891378	-4.355574	0.840221
49	6	2.478637	-2.426140	0.360626
50	1	2.339595	-2.844861	-0.640666
51	1	3.059540	-3.160276	0.934324
52	6	1.272312	2.046750	-2.429776
53	1	1.952610	1.210289	-2.592616
54	1	1.723268	2.932497	-2.897938
55	6	-0.085067	1.779929	-3.081946
56	6	-1.272897	2.046546	2.429638
57	1	-1.952370	1.209389	2.592337
58	1	-1.724765	2.931838	2.897784
59	6	0.084526	1.781056	3.082039
60	6	-1.272574	-2.046716	-2.429509
61	1	-1.952136	-1.209633	-2.592179
62	1	-1.724311	-2.932088	-2.897626
63	6	0.084787	-1.781017	-3.081872
64	6	1.273388	-2.046418	2.429581
65	1	1.953144	-1.209449	2.592093
66	1	1.725133	-2.931824	2.897616
67	6	-0.083862	-1.780518	3.082265
68	1	-0.044296	1.187673	3.990295
69	1	0.595771	2.709741	3.346669
70	1	0.045248	-1.186485	3.990048
71	1	-0.595008	-2.709032	3.347672
72	1	-0.044117	-1.188010	-3.990365
73	1	0.596461	-2.709583	-3.346107
74	1	0.044048	1.185168	-3.989245
75	1	-0.596595	2.708050	-3.347975
76	1	1.812922	-1.011987	-2.457140
77	1	-1.813907	1.013956	-2.455375
78	1	-1.812767	-1.013477	2.457229

79	1	1.813088	1.013221	2.457097

E(RTPSSh) = -1681.3073921 Hartree
Zero-point correction = 0.689838 Hartree/particle
Sum of electronic and thermal Energies = -1680.582193 Hartree
Sum of electronic and thermal Enthalpies = -1680.581249 Hartree
Sum of electronic and thermal Free Energies = -1680.679311 Hartree

Table S20. $[TbL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	65	-0.000102	-0.000038	0.000129
2	7	-2.575068	-0.000120	-0.000454
3	7	-1.120363	2.226135	0.978212
4	7	1.120127	2.226344	-0.978078
5	7	2.575127	0.000146	0.000248
6	7	1.120139	-2.226158	0.978354
7	7	-1.119720	-2.226320	-0.978432
8	8	0.925225	1.039889	2.096675
9	8	-0.925496	1.040131	-2.096403
10	8	-0.925940	-1.039682	2.096461
11	8	0.926112	-1.039781	-2.096021
12	6	-3.262515	-1.141111	-0.244976
13	6	-4.657695	-1.170854	-0.272976
14	1	-5.174456	-2.098610	-0.490954
15	6	-5.363877	-0.000377	-0.000537
16	1	-6.448505	-0.000474	-0.000560
17	6	-4.657918	1.170241	0.271939
18	1	-5.174866	2.097895	0.489901
19	6	-3.262745	1.140763	0.244031
20	6	-2.472886	2.421452	0.399942
21	1	-2.349439	2.860430	-0.594879
22	1	-3.050163	3.142206	0.993715
23	6	-0.286022	3.434366	0.702832
24	1	0.524309	3.459179	1.430525
25	1	-0.877154	4.347196	0.854604
26	6	0.285783	3.434536	-0.702399
27	1	-0.524540	3.459564	-1.430096
28	1	0.876938	4.347382	-0.853964
29	6	2.472709	2.421709	-0.399965
30	1	2.349353	2.860545	0.594934
31	1	3.049834	3.142597	-0.993720
32	6	3.262684	1.141066	-0.244309
33	6	4.657856	1.170661	-0.272532
34	1	5.174670	2.098374	-0.490564
35	6	5.363958	0.000086	-0.000275
36	1	6.448587	0.000053	-0.000491
37	6	4.657904	-1.170452	0.272263
38	1	5.174773	-2.098184	0.490088
39	6	3.262718	-1.140802	0.244581
40	6	2.472845	-2.421479	0.400552
41	1	2.349766	-2.860677	-0.594221
42	1	3.049980	-3.142069	0.994663
43	6	0.285931	-3.434439	0.702733

44	1	-0.524597	-3.459330	1.430201
45	1	0.877073	-4.347234	0.854662
46	6	-0.285485	-3.434557	-0.702657
47	1	0.525044	-3.459513	-1.430122
48	1	-0.876616	-4.347376	-0.854447
49	6	-2.472501	-2.421725	-0.400774
50	1	-2.349495	-2.860881	0.594028
51	1	-3.049496	-3.142410	-0.994905
52	6	-1.232371	2.047851	2.451525
53	1	-1.921061	1.223268	2.635841
54	1	-1.659840	2.943729	2.922501
55	6	0.136718	1.767276	3.073912
56	6	1.231883	2.048337	-2.451437
57	1	1.920671	1.223899	-2.636040
58	1	1.659175	2.944336	-2.922343
59	6	-0.137323	1.767815	-3.073543
60	6	1.231618	-2.047800	2.451693
61	1	1.920207	-1.223170	2.636183
62	1	1.659032	-2.943596	2.922889
63	6	-0.137672	-1.767403	3.073654
64	6	-1.231080	-2.048057	-2.451824
65	1	-1.919768	-1.223542	-2.636442
66	1	-1.658277	-2.943966	-2.922976
67	6	0.138287	-1.767463	-3.073500
68	1	-0.027578	1.175611	-3.984924
69	1	-0.665462	2.690647	-3.324964
70	1	0.028821	-1.175195	-3.984867
71	1	0.666574	-2.690245	-3.324784
72	1	-0.028030	-1.175129	3.985001
73	1	-0.665817	-2.690221	3.325054
74	1	0.026773	1.174682	3.985001
75	1	0.664774	2.690031	3.325728
76	1	-1.847477	-1.000136	2.393694
77	1	1.846539	0.999465	2.394483
78	1	1.847376	-0.998375	-2.393841
79	1	-1.846762	0.999234	-2.394291

E(RTPSSh) = -1681.8966149 Hartree
Zero-point correction = 0.690613 Hartree/particle
Sum of electronic and thermal Energies = -1681.170898 Hartree
Sum of electronic and thermal Enthalpies = -1681.169954 Hartree
Sum of electronic and thermal Free Energies = -1681.267340 Hartree

Table S21. $[DyL^{1}]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	66	0.000037	-0.000076	0.000138
2	7	2.569875	0.000100	0.000058
3	7	1.115472	2.221855	-0.980146
4	7	-1.115684	2.221769	0.980153
5	7	-2.569843	-0.000089	0.000004
6	7	-1.115422	-2.221815	-0.980128
7	7	1.115693	-2.221781	0.980244
8	8	-0.928824	1.030585	-2.082710

9	8	0.928595	1.030598	2.082977
10	8	0.928654	-1.030164	-2.083052
11	8	-0.928735	-1.030698	2.082869
12	6	3.258525	-1.139634	0.247811
13	6	4.653687	-1.169219	0.275771
14	1	5.170092	-2.096533	0.496473
15	6	5.360044	0.000178	-0.000256
16	1	6.444664	0.000209	-0.000383
17	6	4.653554	1.169539	-0.276121
18	1	5.169860	2.096879	-0.496944
19	6	3.258404	1.139881	-0.247848
20	6	2.469420	2.420009	-0.407276
21	1	2.349602	2.863882	0.585838
22	1	3.045053	3.137740	-1.006222
23	6	0.282651	3.430718	-0.703430
24	1	-0.530519	3.455229	-1.427919
25	1	0.873675	4.343004	-0.858574
26	6	-0.282909	3.430674	0.703517
27	1	0.530264	3.455164	1.428006
28	1	-0.873959	4.342934	0.858715
29	6	-2.469619	2.419853	0.407232
30	1	-2.349799	2.863854	-0.585822
31	1	-3.045345	3.137467	1.006231
32	6	-3.258489	1.139670	0.247627
33	6	-4.653655	1.169275	0.275469
34	1	-5.170067	2.096612	0.496064
35	6	-5.360006	-0.000133	-0.000526
36	1	-6.444626	-0.000148	-0.000738
37	6	-4.653513	-1.169527	-0.276251
38	1	-5.169816	-2.096874	-0.497052
39	6	-3.258366	-1.139880	-0.247878
40	6	-2.469353	-2.420003	-0.407204
41	1	-2.349488	-2.863795	0.585938
42	1	-3.044959	-3.137801	-1.006094
43	6	-0.282543	-3.430651	-0.703494
44	1	0.530666	-3.455022	-1.427947
45	1	-0.873493	-4.342963	-0.858758
46	6	0.282968	-3.430708	0.703478
47	1	-0.530220	-3.455307	1.427942
48	1	0.874059	-4.342951	0.858606
49	6	2.469677	-2.419829	0.407410
50	1	2.349936	-2.863862	-0.585641
51	1	3.045381	-3.137416	1.006459
52	6	1.222021	2.045669	-2.454057
53	1	1.915265	1.226225	-2.643440
54	1	1.640856	2.945153	-2.925856
55	6	-0.149437	1.757433	-3.067665
56	6	-1.222335	2.045513	2.454054
57	1	-1.915435	1.225919	2.643334
58	1	-1.641401	2.944889	2.925850
59	6	0.149104	1.757540	3.067790
60	6	-1.222082	-2.045560	-2.454031
61	1	-1.915278	-1.226049	-2.643308
62	1	-1.641027	-2.944989	-2.925833
63	6	0.149317	-1.757403	-3.067760
64	6	1.222207	-2.045558	2.454162
65	1	1.915307	-1.225985	2.643525
66	1	1.641207	-2.944954	2.925975
67	6	-0.149288	-1.757563	3.067779
68	1	0.042939	1.162582	3.977732

69	1	0.682547	2.677279	3.319094
70	1	-0.043199	-1.162548	3.977691
71	1	-0.682730	-2.677298	3.319102
72	1	0.043042	-1.162594	-3.977789
73	1	0.682936	-2.677074	-3.318941
74	1	-0.043249	1.162339	-3.977515
75	1	-0.682976	2.677081	-3.319102
76	1	1.853237	-0.990489	-2.370344
77	1	-1.853361	0.990675	-2.370120
78	1	-1.853227	-0.990647	2.370411
79	1	1.853099	0.990674	2.370495

E(RTPSSh) = -1682.4816153 Hartree
Zero-point correction = 0.691449 Hartree/particle
Sum of electronic and thermal Energies = -1681.755368 Hartree
Sum of electronic and thermal Enthalpies = -1681.754423 Hartree
Sum of electronic and thermal Free Energies = -1681.850770 Hartree

Table S22. $[HoL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	0.000087	-0.000267	0.000357
2	7	2.565244	0.000222	0.000150
3	7	1.111788	2.218075	-0.980183
4	7	-1.112090	2.217725	0.980521
5	7	-2.565248	-0.000087	-0.000096
6	7	-1.111641	-2.217676	-0.980678
7	7	1.112029	-2.217876	0.980262
8	8	-0.930308	1.021845	-2.069894
9	8	0.929929	1.020916	2.071101
10	8	0.930158	-1.020023	-2.070977
11	8	-0.930408	-1.022058	2.070217
12	6	3.254837	-1.138760	0.249135
13	6	4.649977	-1.168507	0.276851
14	1	5.165968	-2.095808	0.498578
15	6	5.356637	0.000241	-0.000632
16	1	6.441246	0.000257	-0.000951
17	6	4.649786	1.168985	-0.277715
18	1	5.165646	2.096283	-0.499751
19	6	3.254678	1.139236	-0.249219
20	6	2.466386	2.418803	-0.410739
21	1	2.348661	2.865872	0.581188
22	1	3.040804	3.134709	-1.013018
23	6	0.280351	3.427655	-0.703780
24	1	-0.534583	3.451733	-1.426329
25	1	0.871556	4.339341	-0.861539
26	6	-0.280952	3.427544	0.704198
27	1	0.534064	3.451771	1.426627
28	1	-0.872345	4.339080	0.862081
29	6	-2.466797	2.418440	0.411337
30	1	-2.349279	2.866185	-0.580305
31	1	-3.041265	3.133873	1.014126
32	6	-3.254872	1.138813	0.249139
33	6	-4.650012	1.168507	0.276889

34	1	-5.166026	2.095761	0.498760
35	6	-5.356647	-0.000227	-0.000723
36	1	-6.441255	-0.000285	-0.000968
37	6	-4.649766	-1.168900	-0.278025
38	1	-5.165602	-2.096193	-0.500141
39	6	-3.254654	-1.139071	-0.249648
40	6	-2.466345	-2.418587	-0.411530
41	1	-2.348810	-2.866093	0.580222
42	1	-3.040633	-3.134229	-1.014241
43	6	-0.280304	-3.427376	-0.704424
44	1	0.534789	-3.451344	-1.426779
45	1	-0.871504	-4.339005	-0.862495
46	6	0.280834	-3.427624	0.703626
47	1	-0.534185	-3.451969	1.426057
48	1	0.872232	-4.339185	0.861316
49	6	2.466763	-2.418428	0.411039
50	1	2.349272	-2.865909	-0.580732
51	1	3.041231	-3.134006	1.013648
52	6	1.215082	2.043218	-2.454292
53	1	1.912696	1.228452	-2.647220
54	1	1.626550	2.945783	-2.926681
55	6	-0.157708	1.747398	-3.061475
56	6	-1.215377	2.042345	2.454660
57	1	-1.912305	1.226892	2.647170
58	1	-1.627698	2.944375	2.927326
59	6	0.157468	1.747625	3.061942
60	6	-1.214824	-2.042108	-2.454793
61	1	-1.911846	-1.226731	-2.647275
62	1	-1.626893	-2.944169	-2.927617
63	6	0.158019	-1.747016	-3.061892
64	6	1.215128	-2.042974	2.454457
65	1	1.912252	-1.227787	2.647380
66	1	1.627112	-2.945292	2.926852
67	6	-0.157828	-1.748061	3.061537
68	1	0.053459	1.150465	3.970619
69	1	0.695672	2.664489	3.313302
70	1	-0.053927	-1.150281	3.969806
71	1	-0.695940	-2.664830	3.313425
72	1	0.053906	-1.149877	-3.970567
73	1	0.696533	-2.663700	-3.313231
74	1	-0.053256	1.148977	-3.969260
75	1	-0.696078	2.663768	-3.314242
76	1	1.857611	-0.982499	-2.349120
77	1	-1.857870	0.985082	-2.347759
78	1	-1.857662	-0.983968	2.348949
79	1	1.857156	0.982737	2.349917

E(RTPSSh) = -1683.0644547 Hartree
Zero-point correction = 0.691946 Hartree/particle
Sum of electronic and thermal Energies = -1682.337880 Hartree
Sum of electronic and thermal Enthalpies = -1682.336935 Hartree
Sum of electronic and thermal Free Energies = -1682.432784 Hartree

Table S23. $[TmL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	69	0.000048	0.000272	-0.000053
2	7	2.556064	-0.000045	-0.000076
3	7	1.103486	-2.210351	0.983744
4	7	-1.103352	-2.210116	-0.983986
5	7	-2.556089	-0.000121	0.000099
6	7	-1.103390	2.209948	0.984154
7	7	1.103300	2.210232	-0.983743
8	8	-0.935929	-1.004992	2.047815
9	8	0.935852	-1.004086	-2.048350
10	8	0.935936	1.003676	2.048446
11	8	-0.936221	1.004930	-2.047803
12	6	3.247072	1.136646	-0.256275
13	6	4.642143	1.166377	-0.285028
14	1	5.157290	2.092645	-0.512954
15	6	5.349481	0.000026	-0.000111
16	1	6.434072	0.000050	-0.000117
17	6	4.642198	-1.166353	0.284825
18	1	5.157394	-2.092595	0.512746
19	6	3.247125	-1.136706	0.256102
20	6	2.460602	-2.415357	0.423770
21	1	2.349273	-2.870512	-0.565219
22	1	3.032256	-3.125979	1.034815
23	6	0.275163	-3.421227	0.705332
24	1	-0.544862	-3.444740	1.422082
25	1	0.866212	-4.331860	0.869174
26	6	-0.275047	-3.421082	-0.705795
27	1	0.545019	-3.444468	-1.422492
28	1	-0.866097	-4.331671	-0.869848
29	6	-2.460521	-2.415330	-0.424184
30	1	-2.349281	-2.870757	0.564688
31	1	-3.032056	-3.125816	-1.035494
32	6	-3.247109	-1.136748	-0.256308
33	6	-4.642180	-1.166450	-0.285087
34	1	-5.157334	-2.092683	-0.513140
35	6	-5.349509	-0.000126	-0.000041
36	1	-6.434101	-0.000126	-0.000101
37	6	-4.642216	1.166197	0.285100
38	1	-5.157403	2.092421	0.513118
39	6	-3.247139	1.136499	0.256469
40	6	-2.460629	2.415114	0.424487
41	1	-2.349518	2.870697	-0.564325
42	1	-3.032159	3.125456	1.035964
43	6	-0.275173	3.420973	0.705908
44	1	0.544923	3.444402	1.422561
45	1	-0.866266	4.331523	0.870012
46	6	0.274989	3.421170	-0.705244
47	1	-0.545054	3.444733	-1.421961
48	1	0.866083	4.331766	-0.869076
49	6	2.460514	2.415278	-0.423924
50	1	2.349328	2.870510	0.565044
51	1	3.032057	3.125859	-1.035108
52	6	1.197647	-2.037724	2.458573
53	1	1.900752	-1.229807	2.658961

54	1	1.596778	-2.944790	2.932798
55	6	-0.178882	-1.730847	3.051408
56	6	-1.197540	-2.037036	-2.458810
57	1	-1.900353	-1.228784	-2.658891
58	1	-1.597022	-2.943808	-2.933297
59	6	0.178993	-1.730532	-3.051648
60	6	-1.197411	2.036767	2.458992
61	1	-1.900100	1.228412	2.659075
62	1	-1.596947	2.943474	2.933555
63	6	0.179199	1.730407	3.051689
64	6	1.197358	2.037607	-2.458622
65	1	1.900363	1.229613	-2.659043
66	1	1.596565	2.944642	-2.932823
67	6	-0.179227	1.730922	-3.051372
68	1	0.080940	-1.129742	-3.958447
69	1	0.726306	-2.642263	-3.301572
70	1	-0.081179	1.129721	-3.957891
71	1	-0.726494	2.642572	-3.301679
72	1	0.081303	1.129836	3.958642
73	1	0.726556	2.642192	3.301309
74	1	-0.080657	-1.129496	3.957811
75	1	-0.726186	-2.642406	3.301961
76	1	1.868321	0.966379	2.309601
77	1	-1.868337	-0.968064	2.308930
78	1	-1.868484	0.967291	-2.309340
79	1	1.868132	-0.966461	-2.309830

E(RTPSSh) = -1684.2248052 Hartree
Zero-point correction = 0.692777 Hartree/particle
Sum of electronic and thermal Energies = -1683.497695 Hartree
Sum of electronic and thermal Enthalpies = -1683.496750 Hartree
Sum of electronic and thermal Free Energies = -1683.591865 Hartree

Table S24. $[YbL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.000034	0.000283	-0.000027
2	7	2.551707	-0.000015	-0.000128
3	7	1.099050	-2.206524	0.986566
4	7	-1.098814	-2.206297	-0.986813
5	7	-2.551729	-0.000172	0.000170
6	7	-1.098915	2.206073	0.987046
7	7	1.098727	2.206398	-0.986593
8	8	-0.939456	-0.996767	2.036661
9	8	0.939471	-0.995811	-2.037109
10	8	0.939611	0.995531	2.037142
11	8	-0.939933	0.996671	-2.036524
12	6	3.243352	1.135257	-0.261299
13	6	4.638406	1.164872	-0.290576
14	1	5.153208	2.090273	-0.522774
15	6	5.346005	0.000110	-0.000209
16	1	6.430589	0.000154	-0.000230
17	6	4.638514	-1.164710	0.290194
18	1	5.153409	-2.090065	0.522368

19	6	3.243457	-1.135234	0.260991
20	6	2.457833	-2.413463	0.432235
21	1	2.350396	-2.873123	-0.555097
22	1	3.027936	-3.120956	1.048304
23	6	0.272077	-3.417776	0.706273
24	1	-0.550919	-3.440925	1.419597
25	1	0.862676	-4.328074	0.873357
26	6	-0.271829	-3.417623	-0.706752
27	1	0.551206	-3.440618	-1.420025
28	1	-0.862414	-4.327883	-0.874065
29	6	-2.457648	-2.413500	-0.432667
30	1	-2.350285	-2.873423	0.554551
31	1	-3.027595	-3.120884	-1.049002
32	6	-3.243393	-1.135370	-0.261241
33	6	-4.638442	-1.164933	-0.290607
34	1	-5.153257	-2.090288	-0.522961
35	6	-5.346029	-0.000185	-0.000139
36	1	-6.430613	-0.000191	-0.000267
37	6	-4.638524	1.164563	0.290504
38	1	-5.153405	2.089908	0.522755
39	6	-3.243460	1.135012	0.261454
40	6	-2.457848	2.413200	0.433101
41	1	-2.350683	2.873364	-0.554024
42	1	-3.027802	3.120360	1.049682
43	6	-0.272042	3.417477	0.706909
44	1	0.551050	3.440520	1.420108
45	1	-0.862679	4.327686	0.874304
46	6	0.271749	3.417697	-0.706161
47	1	-0.551297	3.440887	-1.419414
48	1	0.862373	4.327965	-0.873262
49	6	2.457641	2.413439	-0.432518
50	1	2.350401	2.873222	0.554776
51	1	3.027567	3.120878	-1.048802
52	6	1.187576	-2.035207	2.461869
53	1	1.892973	-1.230537	2.666573
54	1	1.580397	-2.944466	2.937070
55	6	-0.191175	-1.723094	3.046566
56	6	-1.187345	-2.034522	-2.462115
57	1	-1.892499	-1.229557	-2.666525
58	1	-1.580451	-2.943512	-2.937591
59	6	0.191408	-1.722683	-3.046784
60	6	-1.187228	2.034231	2.462366
61	1	-1.892298	1.229212	2.666835
62	1	-1.580334	2.943188	2.937901
63	6	0.191620	1.722505	3.046855
64	6	1.187053	2.035115	-2.461961
65	1	1.892396	1.230426	-2.666768
66	1	1.579855	2.944384	-2.937141
67	6	-0.191774	1.723100	-3.046488
68	1	0.097500	-1.120630	-3.953108
69	1	0.743301	-2.632112	-3.294838
70	1	-0.097903	1.120649	-3.952542
71	1	-0.743632	2.632450	-3.294894
72	1	0.097884	1.120527	3.953238
73	1	0.743509	2.631978	3.294742
74	1	-0.097100	-1.120556	3.952546
75	1	-0.743027	-2.632390	3.295179
76	1	1.874362	0.957258	2.289557
77	1	-1.874197	-0.958715	2.289138
78	1	-1.874557	0.957954	-2.289337

79	1	1.874096	-0.957068	-2.289919

E(RTPSSh) = -1684.8066586 Hartree
Zero-point correction = 0.693244 Hartree/particle
Sum of electronic and thermal Energies = -1684.079236 Hartree
Sum of electronic and thermal Enthalpies = -1684.078292 Hartree
Sum of electronic and thermal Free Energies = -1684.172938 Hartree

Table S25. $[LuL^1]^{3+}$, TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	0.000041	0.000022	-0.000032
2	7	2.547794	-0.000027	-0.000053
3	7	1.095108	-2.202720	0.988463
4	7	-1.095250	-2.202819	-0.988256
5	7	-2.547816	0.000040	-0.000011
6	7	-1.095187	2.202697	0.988306
7	7	1.095229	2.202744	-0.988446
8	8	-0.942157	-0.989348	2.027318
9	8	0.942146	-0.990034	-2.027113
10	8	0.942202	0.989894	2.027092
11	8	-0.942084	0.989601	-2.027334
12	6	3.240298	1.134059	-0.264636
13	6	4.635361	1.163522	-0.294109
14	1	5.149883	2.088358	-0.529222
15	6	5.343127	-0.000106	0.000006
16	1	6.427711	-0.000137	0.000027
17	6	4.635282	-1.163691	0.294109
18	1	5.149744	-2.088550	0.529259
19	6	3.240222	-1.134152	0.264584
20	6	2.455278	-2.411863	0.438945
21	1	2.351274	-2.875889	-0.546698
22	1	3.023814	-3.116454	1.059747
23	6	0.269427	-3.414676	0.707315
24	1	-0.555815	-3.437618	1.418014
25	1	0.860014	-4.324424	0.877182
26	6	-0.269564	-3.414747	-0.706991
27	1	0.555666	-3.437740	-1.417705
28	1	-0.860149	-4.324515	-0.876764
29	6	-2.455420	-2.411852	-0.438721
30	1	-2.351440	-2.875760	0.546980
31	1	-3.023975	-3.116502	-1.059440
32	6	-3.240301	-1.134080	-0.264530
33	6	-4.635363	-1.163557	-0.294068
34	1	-5.149864	-2.088414	-0.529140
35	6	-5.343159	0.000082	-0.000066
36	1	-6.427744	0.000099	-0.000090
37	6	-4.635342	1.163695	0.293979
38	1	-5.149821	2.088565	0.529048
39	6	-3.240279	1.134167	0.264497
40	6	-2.455341	2.411880	0.438793
41	1	-2.351339	2.875869	-0.546868
42	1	-3.023861	3.116502	1.059577
43	6	-0.269423	3.414591	0.707170

44	1	0.555822	3.437445	1.417874
45	1	-0.859937	4.324383	0.877067
46	6	0.269549	3.414665	-0.707148
47	1	-0.555702	3.437682	-1.417834
48	1	0.860134	4.324432	-0.876926
49	6	2.455415	2.411814	-0.438954
50	1	2.351458	2.875819	0.546704
51	1	3.023968	3.116402	-1.059745
52	6	1.179366	-2.032574	2.464204
53	1	1.887014	-1.230964	2.672528
54	1	1.566828	-2.943845	2.939865
55	6	-0.201007	-1.716248	3.042280
56	6	-1.179517	-2.032881	-2.464005
57	1	-1.887035	-1.231194	-2.672487
58	1	-1.567099	-2.944174	-2.939529
59	6	0.200929	-1.716865	-3.042069
60	6	-1.179473	2.032578	2.464037
61	1	-1.886912	1.230784	2.672396
62	1	-1.567163	2.943773	2.939660
63	6	0.200989	1.716656	3.042094
64	6	1.179462	2.032758	-2.464199
65	1	1.887080	1.231149	-2.672637
66	1	1.566943	2.944065	-2.939779
67	6	-0.200930	1.716537	-3.042271
68	1	0.110669	-1.113674	-3.947931
69	1	0.756179	-2.624623	-3.288641
70	1	-0.110578	1.113360	-3.948135
71	1	-0.756309	2.624211	-3.288866
72	1	0.110789	1.113423	3.947935
73	1	0.756189	2.624441	3.288686
74	1	-0.110616	-1.113003	3.948095
75	1	-0.756421	-2.623878	3.288963
76	1	1.878488	0.950390	2.273695
77	1	-1.878367	-0.949431	2.274146
78	1	-1.878325	0.949861	-2.274072
79	1	1.878396	-0.950386	-2.273833

```
 E(RTPSSh) = -1685.3592649 Hartree
 Zero-point correction = 0.693803 Hartree/particle
 Sum of electronic and thermal Energies = -1684.631469 Hartree
 Sum of electronic and thermal Enthalpies = -1684.630524 Hartree
 Sum of electronic and thermal Free Energies = -1684.724580 Hartree
```

References

(1) K. Djanashvili, C. Platas-Iglesias, J. A. Peters, *Dalton Trans.* **2008**, 602-607.