Supporting Information

Fluoride Binding in Unlikely Partners: The Formation of Anion-Anion Complexes with $[M(EGTA)]^-$ and $[M(OBETA)]^-$ ($M = Gd^{3+}, Y^{3+}$)

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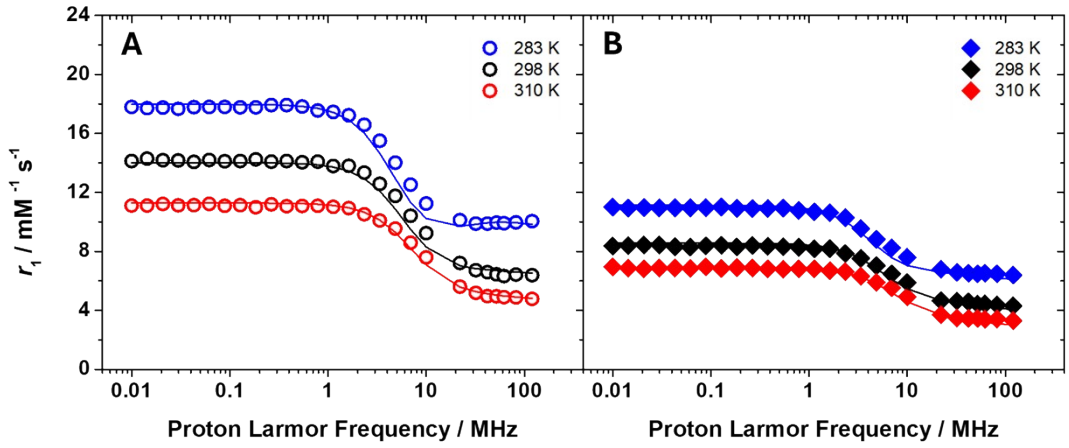

Figure S1. ^{1}H NMRD profiles of an aqueous solution of (A) $[Gd(OBETA)(H_2O)_2]^-$ (2.9 mM and pH = 7.15) and (B) $[Gd(EGTA)(H_2O)]^-$ (5.2 mM and pH = 7.15) recorded at 283 K (**blue**), 298 K (**black**) and 310 K (**red**). The solid lines correspond to the fits of the data, as described in the text.

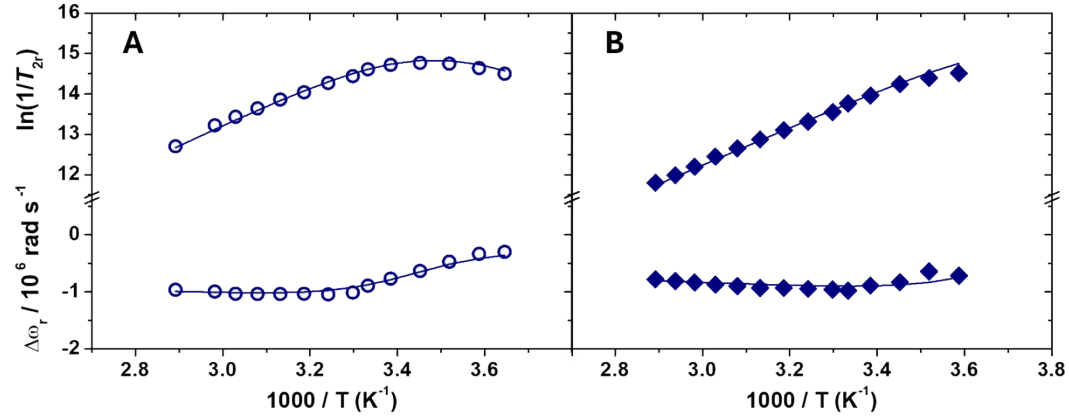

Figure S2. ^{17}O transverse relaxation rates (top) and ^{17}O chemical shift variation (bottom) as a function of the temperature of (A) $[Gd(OBETA)(H_2O)_2]^-$ (7.0 mM and pH = 7.0)[1] and (B) $[Gd(EGTA)(H_2O)]^-$ (32 mM and pH = 7.0) measured at 11.75 T. The solid lines correspond to the fits of the data, as described in the text.

Table S1. Parameters Obtained from the Simultaneous Analysis of ^{1}H NMRD Profiles and ^{17}O NMR Data (11.75 T) for the Gd^{3+} Complexes of OBETA and EGTA.

Parameters	$[Gd(OBETA)(H_2O)_2]^-$	$[Gd(OBETA)(H_2O)F]^{2-}$	$[Gd(EGTA)(H_2O)]^-$	$[Gd(EGTA)F]^{2-}$
$^{298}r_1$ / mM^{-1} s^{-1} (1.5 T)	6.3	4.9	4.4	3.5
$^{298}\Delta^2$/ 10^{19} s^{-2}	4.3 ± 0.1	5.7 ± 0.1	3.2 ± 0.1	2.6 ± 0.1
$^{298}\tau_V$ / ps	16.4 ± 0.1	20.0 ± 1.0	26.0 ± 1.0	31.5 ± 0.3
E_V / kJ mol^{-1}	1.0 [a]	1.0 [a]	1.0 [a]	1.0 [a]
$^{298}k_{ex}$ / 10^6 s^{-1}	13.0 ± 1	15.0 ± 0.1	55.0 ± 2.0	//
ΔH_M / kJ mol^{-1}	40.0 ± 3.5	36.0 ± 1.6	36.1 ± 0.9	//
$A_O/\hbar$ (10^6 rad/s)	– 2.9 ± 0.2	– 3.5 ± 0.1	– 3.3 ± 0.4	//
C_{os}	0.3	0.0	0.0 [a]	//
$^{298}\tau_R$/ ps	63 ± 1	66 ± 1	64 ± 1	//
E_R / kJ mol^{-1}	18.0 ± 0.1	21.7 ± 0.7	19.8 ± 0.2	//
$^{298}\tau_R^{SS}$/ ps	//	41.5 ± 0.1	//	59.8 ± 0.7
E_R^{SS} / kJ mol^{-1}	//	15.0 ± 2.5	//	15.0 ± 1
q	2 [a]	1 [a]	1 [a]	0 [a]
q^{SS}	//	1 [a]	//	2 [a]
r / Å	3.0 [a]	3.0 [a]	3.0 [a]	//
r^{SS} / Å	//	3.6 [a]	//	3.6 [a]
a / Å	4.0 [a]	4.0 [a]	4.0 [a]	4.0 [a]
^{298}D / 10^5 cm^2 s^{-1}	2.24 [a]	2.24 [a]	2.24 [a]	2.24 [a]
E_D / kJ mol^{-1}	29.0	29.0 [a]	22.0	22.0 [a]

[a] Parameters fixed during the fitting procedures.

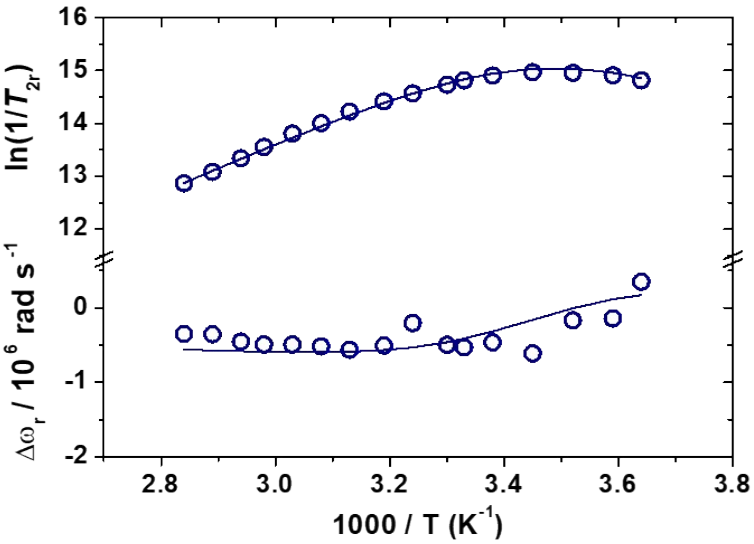

Figure S3. Calculated ^{17}O transverse relaxation rates (top) and ^{17}O chemical shift variation (bottom) as a function of temperature for $[Gd(OBETA)(H_2O)F]^{2-}$, measured at 11.75 T. The solution was prepared as follows: $[Gd(OBETA)(H_2O)_2]^-$ = 0.5 mM, [NaF] = 0.5 M, [HEPES] = 10 mM, pH 7.5. The contribution to the ^{17}O transverse relaxation rates and chemical shift of the residual $[Gd(OBETA)(H_2O)_2]^-$ species were subtracted, for each temperature, as described in the main text. The solid lines correspond to the fits of the data.

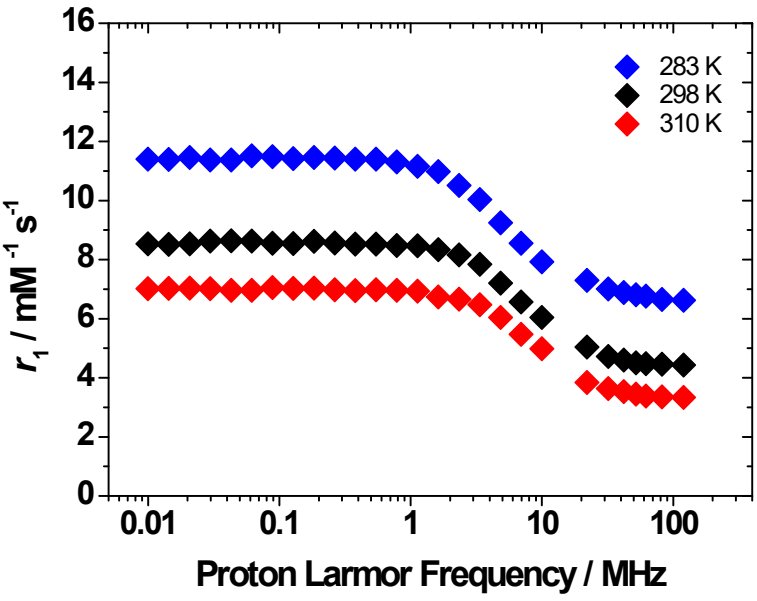

Figure S4. ^1H NMRD profiles of a 0.8 mM solution of $[Gd(EGTA)(H_2O)]^-$ in the presence of NaCl 0.1 M, recorded at different temperatures 283 K (♦), 298 K (♦) and 310 K (♦).

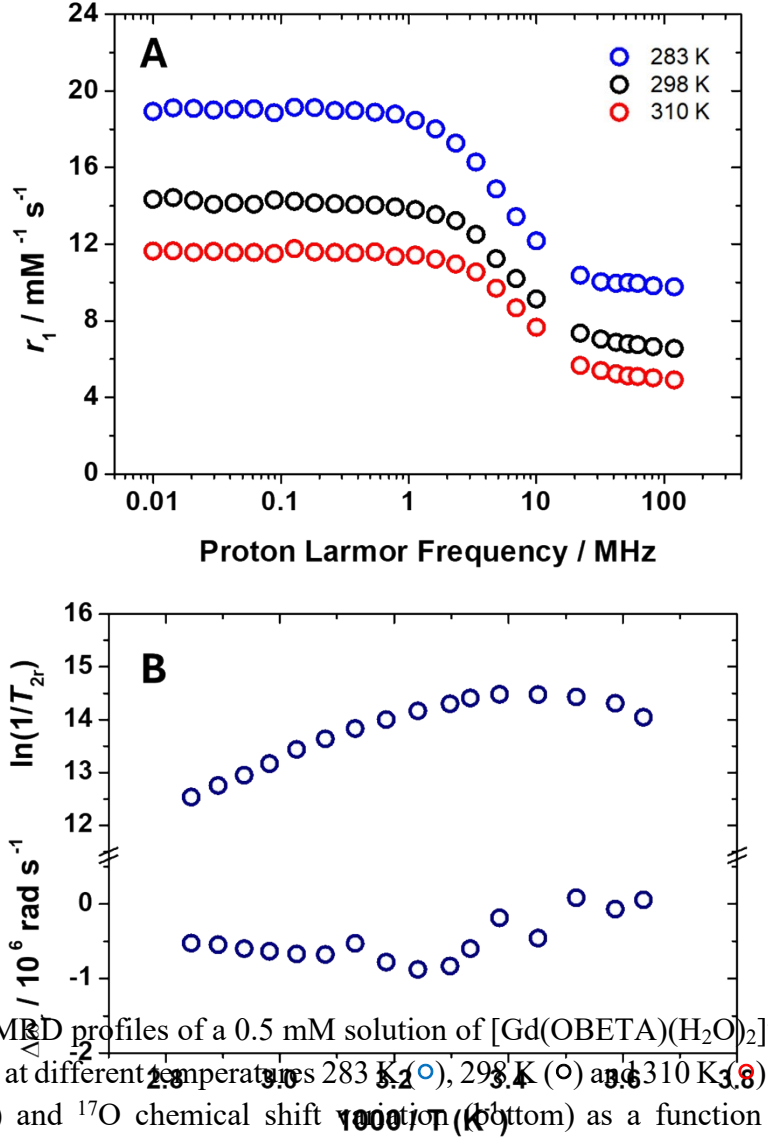

Figure S5. (A) ^{1}H NMRD profiles of a 0.5 mM solution of $[Gd(OBETA)(H_2O)_2]^-$ in the presence of NaCl 0.5 M, recorded at different temperatures 283 K (○), 298 K (○) and 310 K (○). (B) ^{17}O transverse relaxation rates (top) and ^{17}O chemical shift variation (bottom) as a function of temperature of $[Gd(OBETA)(H_2O)_2]^-$ 9.0 mM, in the presence of NaCl 0.07 M, measured at 11.75 T. The solid lines correspond to the fits of the data.

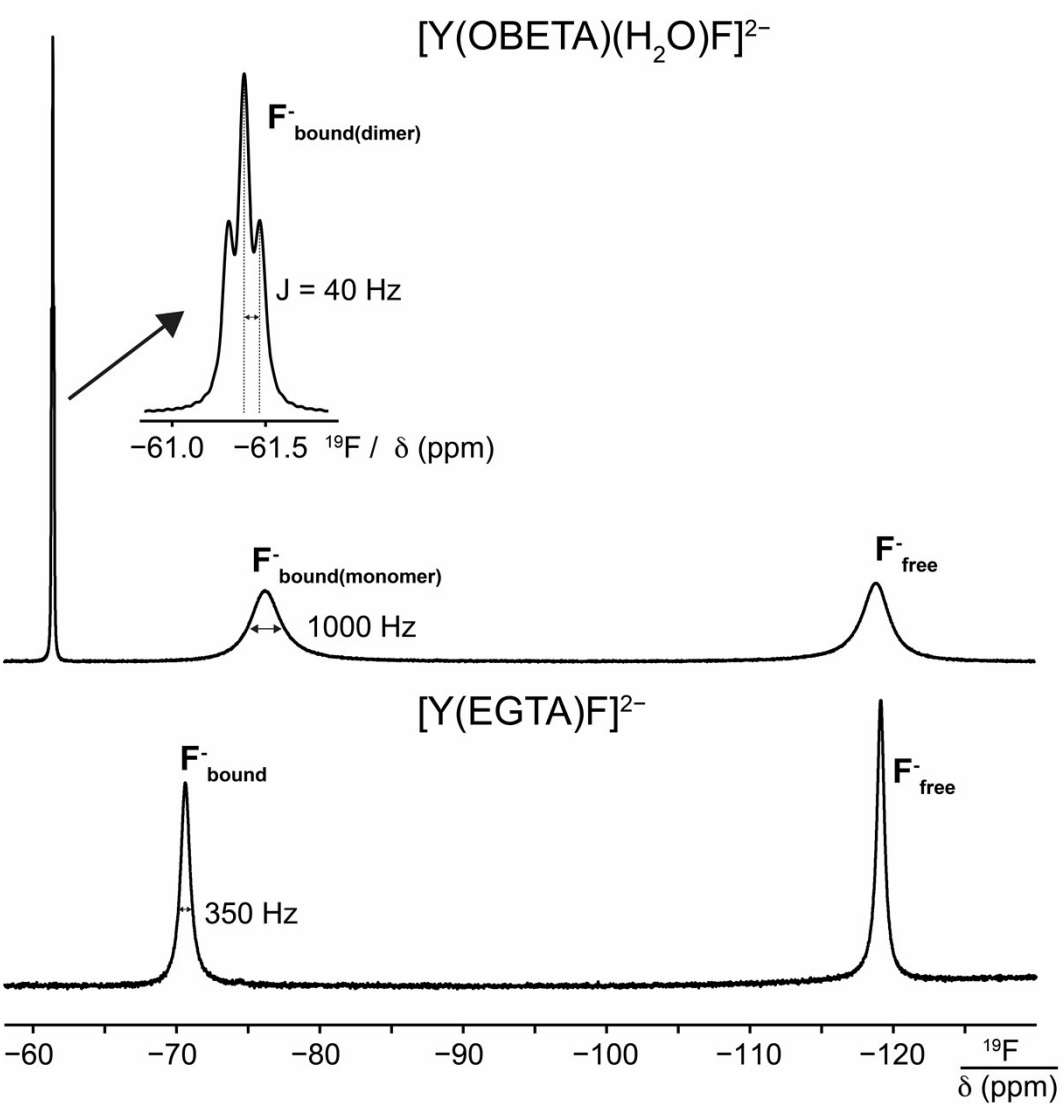

Figure S6. 1D $^{19}F\{^{1}H\}$ NMR spectra of the $[Y(OBETA)(H_2O)F]^{2-}$ (top) and $[Y(EGTA)F]^{2-}$ (bottom) complexes (H_2O/D_2O 9:1, 275 K, 11.75 T). The adducts were prepared by adding NaF (175 mM) to a solution of $[Y(OBETA)(H_2O)_2]^{-}$ (180 mM), and NaF (50 mM) to a solution of $[Y(EGTA)(H_2O)]^{-}$ (200 mM), respectively.

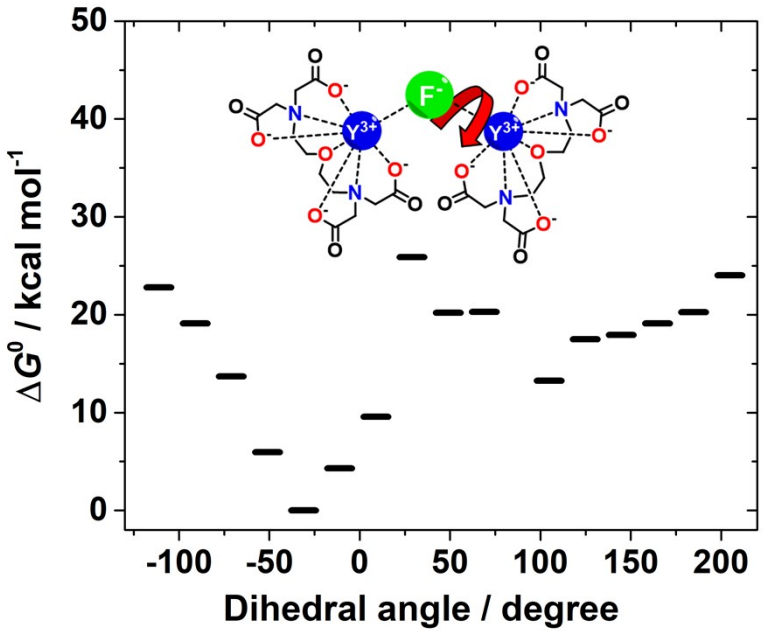

Figure S7. Potential energy surface scan for the O-Y-F-Y dihedral angle involving a carboxylate oxygen atom for $[F\subset(YOBETA)_2]^{3-}$.

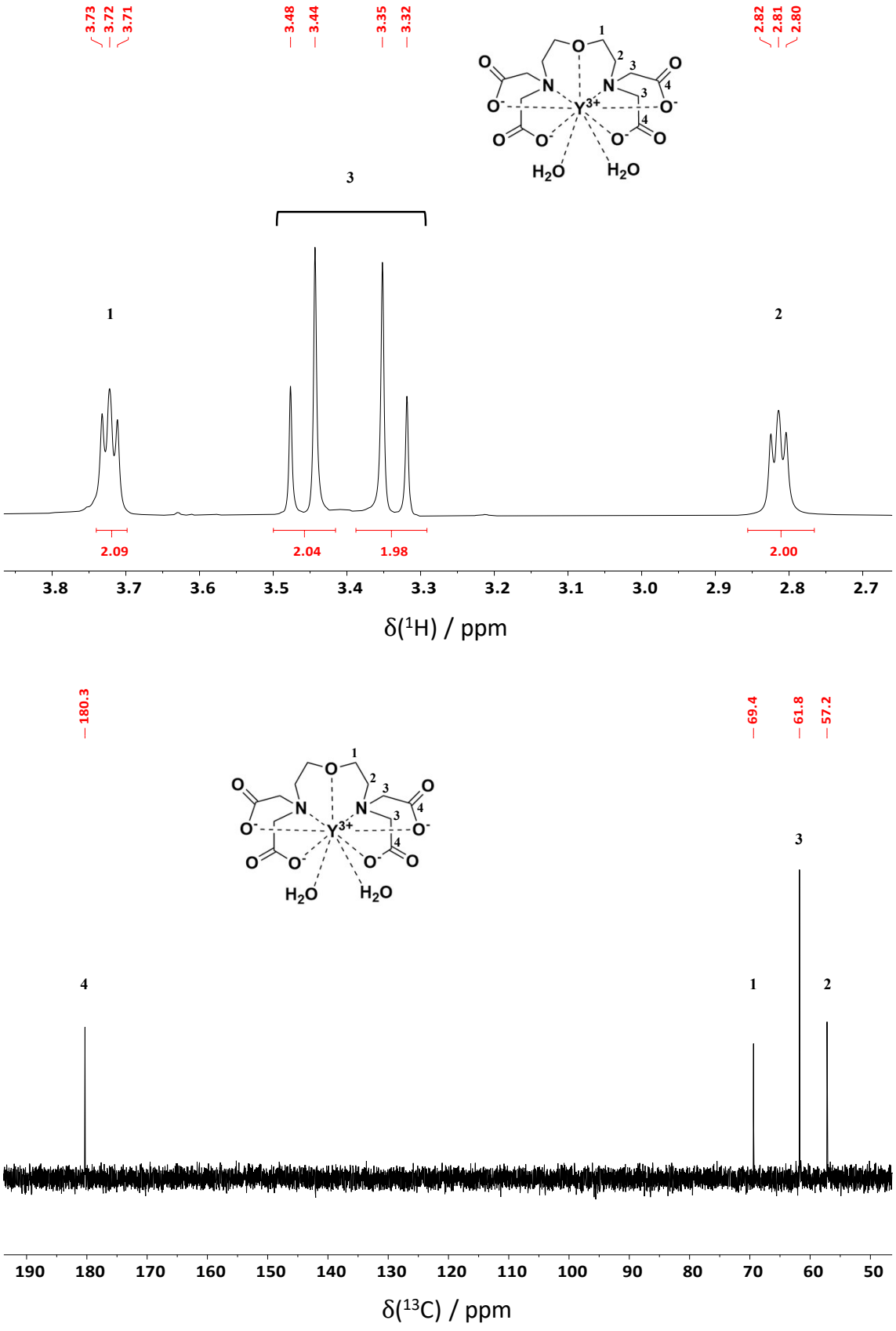

Figure S8. 1D NMR ^{1}H and ^{13}C spectra acquired on a 29.8 mM $[Y(OBETA)(H_2O)_2]^-$ complex at 11.75 T (D_2O, 300 K).

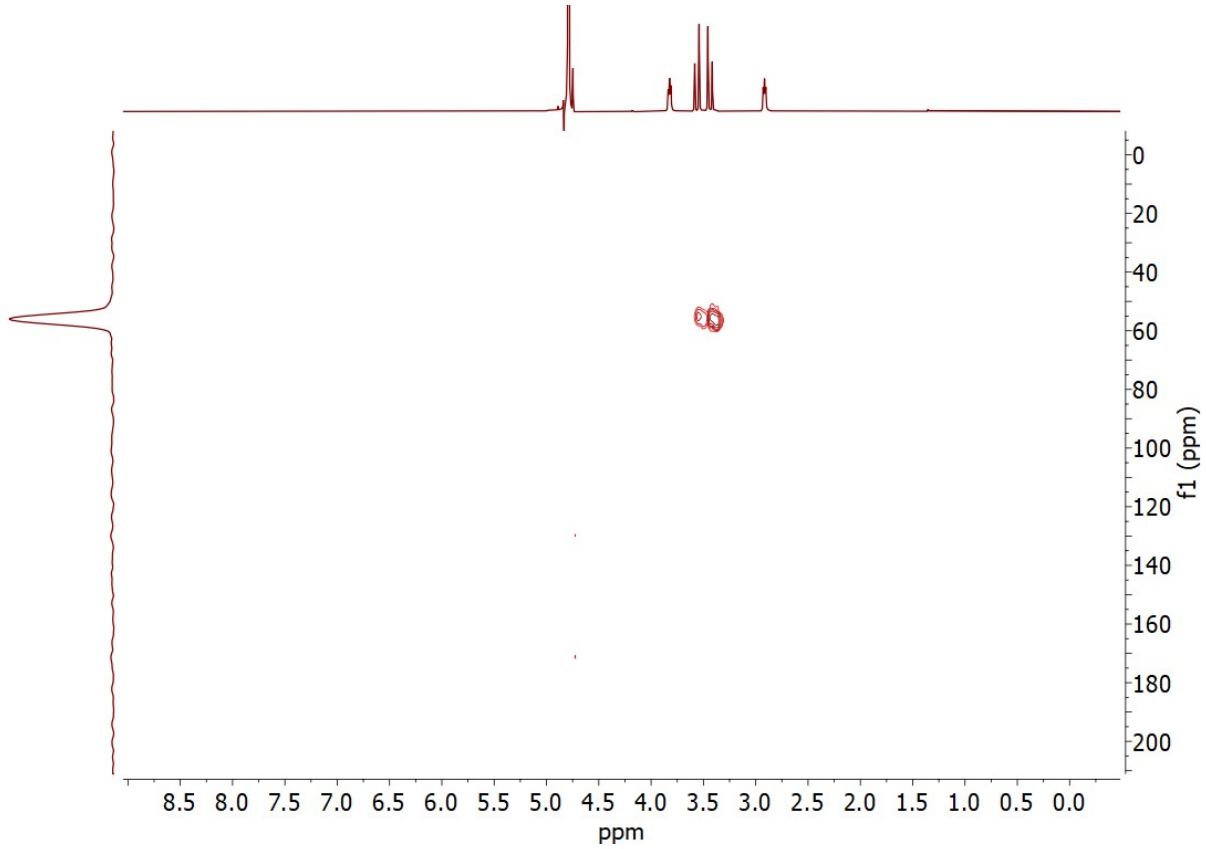

Figure S9. 2D NMR ^{1}H – ^{89}Y HMBC spectrum acquired on a 30 mM $[Y(OBETA)(H_2O)_2]^-$ complex at 9.4 T (D_2O, 298 K).

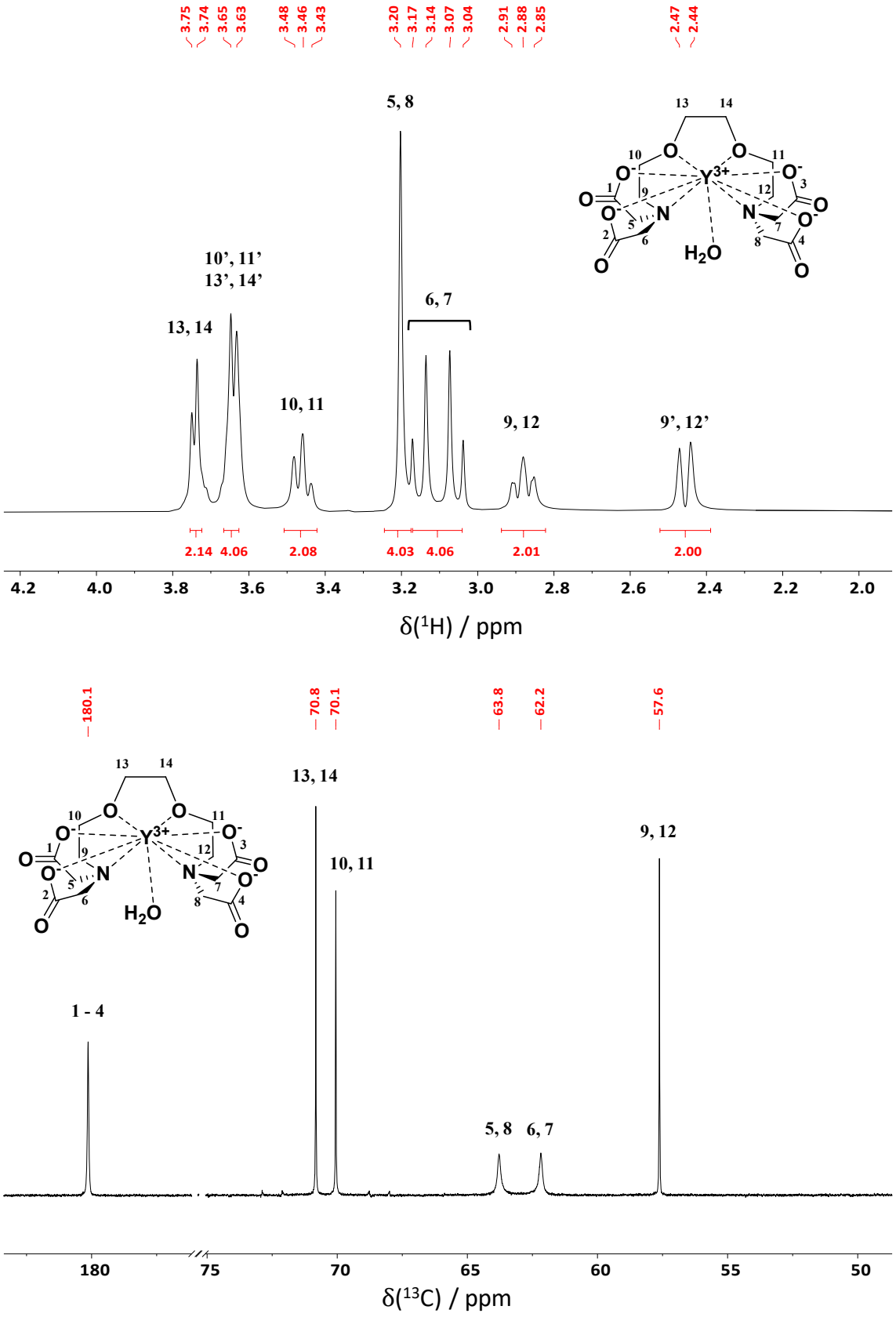

Figure S10. 1D NMR ^{1}H and ^{13}C spectra acquired on a 200 mM $[Y(EGTA)(H_2O)]^-$ complex at 11.75 T (9:1 H_2O/D_2O, 275 K).

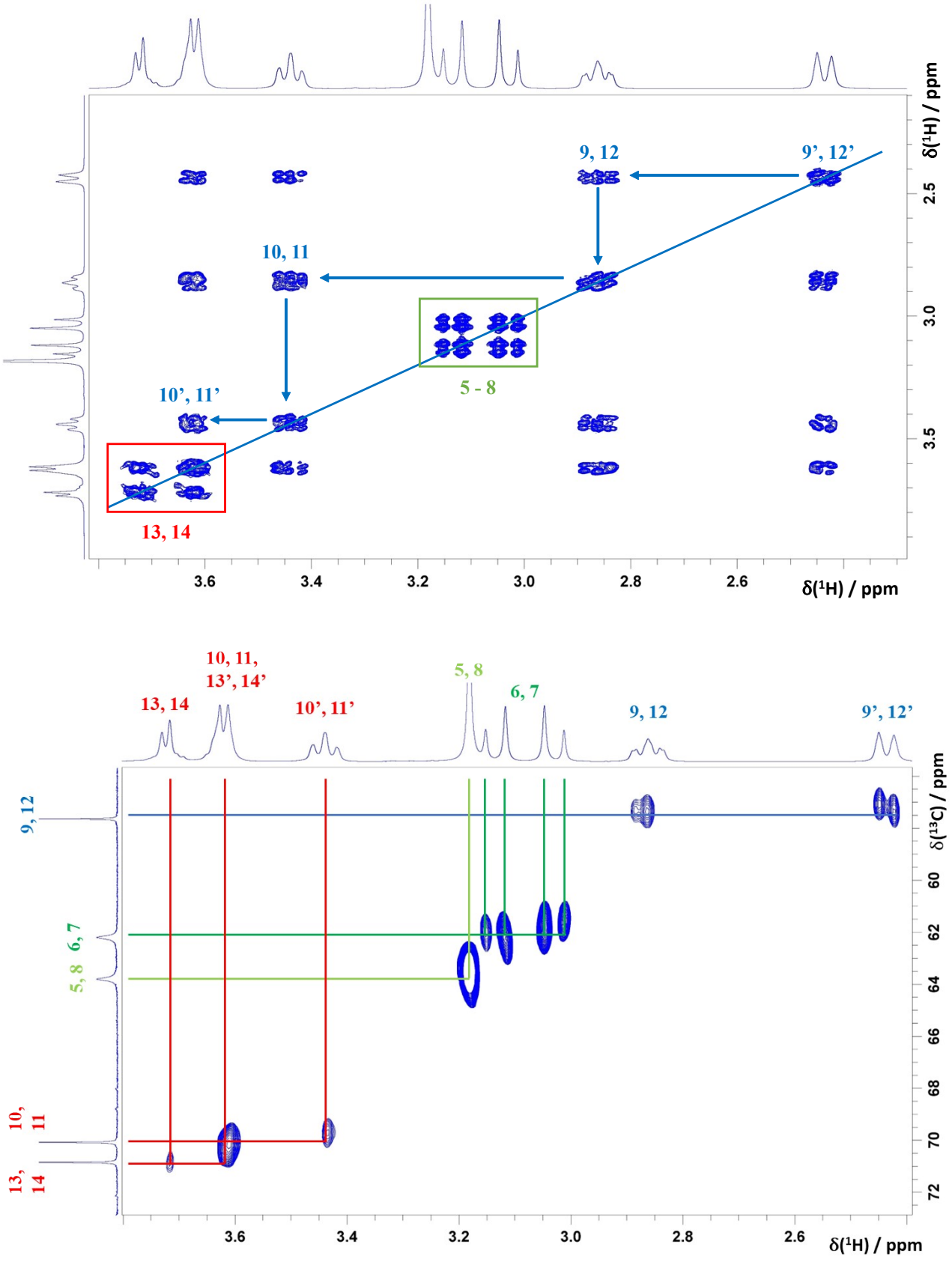

Figure S11. 2D NMR ^{1}H - ^{1}H COSY (top) and ^{1}H - ^{13}C HSQC (bottom) spectra acquired on a 200 mM $[Y(EGTA)(H_2O)]^-$ complex at 11.75 T (9:1 H_2O/D_2O, 275 K).

Table S2. Optimized Cartesian coordinates (Å) of the $[Y(EGTA)(H_2O)]^{-}\cdot 2H_2O$ system obtained with DFT calculations (0 Imaginary Frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.402434	0.197057	1.996694
2	6	0.654339	-0.0745	3.198612
3	8	-1.33474	0.598681	1.985008
4	6	2.705316	-0.42622	1.950723
5	6	2.669111	-1.68126	1.100752
6	6	-2.54015	-0.15435	2.176988
7	6	-3.29236	-0.10169	0.865794
8	7	-2.53223	-0.67199	-0.27014
9	1	0.369701	-1.12979	3.223392
10	1	3.031321	-0.66109	2.966225
11	1	1.947703	-2.3815	1.52142
12	1	-2.30523	-1.17497	2.490089
13	1	-3.49519	0.946883	0.636408
14	6	-3.07672	-0.12631	-1.52859
15	6	-2.52364	-2.1426	-0.23196
16	1	1.2733	0.16402	4.069025
17	1	3.386689	0.32184	1.540128
18	1	-3.14122	0.323698	2.956637
19	1	-4.25811	-0.61272	0.978954
20	7	2.231143	-1.36783	-0.27355
21	1	3.66354	-2.15073	1.110585
22	6	1.831283	-2.57462	-1.01487
23	6	3.267809	-0.61452	-1.01293
24	6	-2.52232	1.286816	-1.73458
25	6	-1.41676	-2.70551	0.670273
26	8	-3.25883	2.212951	-2.12336
27	8	-1.28015	1.415957	-1.47391
28	8	-1.52194	-3.87233	1.071541
29	8	-0.43078	-1.92056	0.906059
30	6	0.821327	-2.25934	-2.12971
31	6	3.00815	0.89058	-1.0128
32	8	3.963677	1.691576	-1.0424
33	8	1.782169	1.230682	-1.01195
34	8	0.734259	-3.04774	-3.08127
35	8	0.101286	-1.21013	-1.9641
36	1	-2.71436	-0.74241	-2.35421
37	1	-4.17186	-0.12372	-1.54361
38	1	-3.4933	-2.55236	0.0745
39	1	-2.31002	-2.50725	-1.23903
40	1	2.692573	-3.10385	-1.43724
41	1	1.3269	-3.2498	-0.32077

42	1	4.270241	-0.83376	-0.63215
43	1	3.243183	-0.92358	-2.06171
44	6	-0.55432	0.830756	3.172825
45	1	-0.24158	1.873579	3.128636
46	1	-1.16914	0.666346	4.060518
47	8	0.101953	2.609762	0.68805
48	1	-0.57994	3.126259	0.203781
49	1	0.964032	3.000523	0.42326
50	8	2.660129	3.874197	0.141988
51	8	-1.95475	4.217672	-0.58042
52	1	2.569189	4.613009	-0.47309
53	1	3.129258	3.16929	-0.36999
54	1	-1.5714	4.923806	-1.11612
55	1	-2.36057	3.59495	-1.22874
56	39	0.003787	0.124011	-0.09538

Table S3. Optimized Cartesian coordinates (Å) of the $[Y(EGTA)(F)]^{2-}\cdot 2H_2O$ system obtained with DFT calculations (0 Imaginary Frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.337982	0.250944	1.940241
2	6	0.840577	1.0377	3.031157
3	8	-1.3226	0.707494	2.084619
4	6	2.68647	-0.22833	2.007934
5	6	2.717594	-1.53835	1.244979
6	6	-2.63337	0.149847	2.171493
7	6	-3.26763	0.237861	0.800205
8	7	-2.55788	-0.54757	-0.23385
9	1	1.45014	0.866573	3.922054
10	1	2.963011	-0.40283	3.051412
11	1	2.029195	-2.22919	1.731101
12	1	-2.57539	-0.88311	2.532891
13	1	-3.26755	1.283655	0.482407
14	6	-3.09603	-0.17773	-1.55577
15	6	-2.65751	-1.99405	0.023435
16	1	0.874592	2.091923	2.751837
17	1	3.366651	0.521403	1.588494
18	1	-3.23302	0.727322	2.884696
19	1	-4.31483	-0.08935	0.875585
20	7	2.259691	-1.36499	-0.14675
21	1	3.732103	-1.9602	1.288059
22	6	1.83298	-2.63882	-0.74616
23	6	3.296304	-0.71356	-0.97599

24	6	-2.47717	1.13485	-2.04758
25	6	-1.53458	-2.53179	0.920324
26	8	-3.16422	1.932966	-2.70844
27	8	-1.24813	1.297116	-1.74566
28	8	-1.70257	-3.64415	1.450067
29	8	-0.49137	-1.80604	1.018264
30	6	0.833056	-2.44079	-1.89745
31	6	3.036257	0.775046	-1.20798
32	8	4.002126	1.549721	-1.35871
33	8	1.812227	1.112803	-1.2668
34	8	0.745761	-3.34319	-2.74737
35	8	0.126468	-1.37586	-1.86715
36	1	-2.80329	-0.95015	-2.27058
37	1	-4.19007	-0.10934	-1.55111
38	1	-3.63128	-2.26864	0.447165
39	1	-2.55845	-2.51663	-0.9305
40	1	2.683391	-3.23437	-1.0989
41	1	1.307386	-3.2148	0.017805
42	1	4.294594	-0.86362	-0.55258
43	1	3.293769	-1.17621	-1.96745
44	6	-0.57744	0.58519	3.298979
45	1	-1.02997	1.2086	4.079307
46	1	-0.58668	-0.46134	3.622756
47	8	2.496766	3.66939	0.155623
48	8	-1.68175	4.041759	-0.63738
49	1	1.640096	3.188342	0.234563
50	1	3.01525	3.091064	-0.43458
51	1	-1.01941	3.424695	-0.23894
52	1	-2.02519	3.524974	-1.3834
53	39	0.009623	0.191813	-0.13861
54	9	0.112711	2.361369	0.449305

Table S4. Optimized Cartesian coordinates (Å) of the $[Y(OBETA)(H_2O)_2]^{-}\cdot 4H_2O$ system obtained with DFT calculations (0 Imaginary Frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.384892	-0.42024	-3.44889
2	6	1.564779	0.447948	-3.07811
3	7	2.010083	0.164391	-1.69577
4	6	2.893434	-1.01338	-1.65592
5	1	3.948704	-0.73991	-1.7526
6	1	2.655592	-1.66284	-2.50302

7	6	2.659669	1.35311	-1.12729
8	1	3.22853	1.054472	-0.24321
9	1	3.373612	1.808209	-1.82521
10	1	2.385861	0.311752	-3.79351
11	1	1.245036	1.489547	-3.12214
12	1	-3.83611	2.320337	0.099675
13	6	-2.78116	2.038733	-0.00725
14	7	-2.59359	0.777511	-0.73848
15	1	-2.27913	2.838544	-0.55505
16	6	-2.70427	0.956698	-2.19608
17	6	-3.51602	-0.25989	-0.24145
18	6	-1.98685	-0.15141	-2.93944
19	1	-2.22694	1.90326	-2.45341
20	1	-3.75334	1.001338	-2.52086
21	1	-3.82613	0.000172	0.772776
22	1	-4.428	-0.31171	-0.8483
23	8	-0.63027	-0.1455	-2.47595
24	1	-2.00763	0.055931	-4.0123
25	1	-2.43072	-1.13527	-2.76507
26	1	0.624808	-1.48905	-3.44032
27	1	0.025272	-0.1549	-4.44614
28	6	1.641253	2.41583	-0.68527
29	6	2.68732	-1.86722	-0.40746
30	6	-2.12033	1.960663	1.36912
31	6	-2.89983	-1.65468	-0.14126
32	8	-1.39117	0.938268	1.589053
33	8	-2.29227	2.891381	2.179631
34	8	-3.65102	-2.59882	0.177255
35	8	-1.64595	-1.758	-0.33569
36	8	1.565795	-1.73642	0.189111
37	8	3.58535	-2.6622	-0.08155
38	8	0.420165	2.058088	-0.61818
39	8	2.085796	3.541444	-0.38376
40	8	-0.20715	-1.66008	2.121809
41	8	1.370539	0.76337	1.880575
42	1	-0.86874	-2.39139	2.071598
43	1	0.63692	-2.06686	1.856862
44	1	2.187073	1.309397	1.836162
45	1	0.786999	1.274389	2.490746
46	8	-0.01427	2.459922	3.71364
47	8	3.527558	2.61062	1.790614
48	1	0.42505	3.316654	3.788843
49	1	-0.86366	2.640891	3.235505
50	1	3.142963	3.144335	1.057991
51	1	3.465364	3.167316	2.577702
52	8	3.138162	-4.22508	2.135949

53	8	-2.07838	-3.76584	2.078115
54	1	-2.65901	-3.48355	1.32512
55	1	-1.64016	-4.57076	1.773427
56	1	3.251805	-3.65496	1.335177
57	1	2.259687	-4.61144	2.035931
58	39	-0.10102	-0.11496	0.018821

Table S5. Optimized Cartesian coordinates (Å) of the $[Y(OBETA)(H_2O)(F)]^{2-}\cdot 4H_2O$ system obtained with DFT calculations (0 Imaginary Frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.02022	-1.88081	2.611941
2	6	-2.25832	-1.05204	2.33551
3	7	-2.41067	-0.66536	0.914753
4	6	-3.05517	-1.71762	0.117601
5	1	-3.57098	-1.25369	-0.7267
6	1	-3.81044	-2.27191	0.689052
7	6	-3.09487	0.629309	0.842262
8	1	-3.50618	0.759446	-0.161
9	1	-3.93564	0.706384	1.54339
10	1	-3.15137	-1.59045	2.682982
11	1	-2.17255	-0.13346	2.91781
12	1	2.979956	2.716064	1.570686
13	6	2.051595	2.221231	1.257232
14	7	2.063435	0.77477	1.505659
15	1	1.226608	2.665714	1.814895
16	6	1.737489	0.432507	2.897851
17	6	3.338033	0.181318	1.062921
18	6	1.237141	-0.99564	3.012616
19	1	0.939932	1.101011	3.224615
20	1	2.601079	0.569321	3.565929
21	1	3.857378	0.892321	0.417314
22	1	4.00378	-0.01066	1.913843
23	8	0.101116	-1.12017	2.14898
24	1	0.938175	-1.19663	4.044695
25	1	1.996182	-1.72686	2.719053
26	1	-1.03402	-2.84658	2.102759
27	1	-0.93377	-2.04973	3.688534
28	6	-2.12561	1.795546	1.090264
29	6	-2.04507	-2.70201	-0.4838
30	6	1.785402	2.507575	-0.22271
31	6	3.189107	-1.10676	0.252445

32	8	1.428856	1.522073	-0.94168
33	8	1.896705	3.683076	-0.63541
34	8	4.229462	-1.65273	-0.16639
35	8	2.007421	-1.51764	0.029043
36	8	-0.81613	-2.39746	-0.37131
37	8	-2.49133	-3.69872	-1.08664
38	8	-0.88562	1.538543	1.068125
39	8	-2.6336	2.930241	1.251358
40	8	-1.31994	1.269261	-1.85492
41	1	-2.08659	1.856028	-1.67835
42	1	-0.6451	1.891561	-2.20582
43	8	0.269531	3.482278	-2.86471
44	8	-3.45883	3.138297	-1.35912
45	1	-0.26727	4.284914	-2.86248
46	1	0.903168	3.589529	-2.10761
47	1	-3.27552	3.246139	-0.3957
48	1	-3.20308	3.97634	-1.76551
49	8	2.999702	-1.78464	-2.88094
50	1	3.447065	-1.8849	-2.01991
51	1	2.104494	-1.45751	-2.63425
52	39	0.100517	-0.24242	-0.17799
53	9	0.503739	-0.83789	-2.26652
54	8	-0.84834	-2.89283	-3.44527
55	1	-1.33787	-3.31296	-2.71414
56	1	-0.35975	-2.16208	-3.00059

Table S6. Optimized Cartesian coordinates (Å) of the $[Y(OBETA)(F)_2]^{2-}\cdot 4H_2O$ system obtained with DFT calculations (0 Imaginary Frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.06239	-1.37975	2.861117
2	6	-2.21599	-0.44412	2.562373
3	7	-2.42821	-0.22662	1.119889
4	6	-3.22195	-1.29318	0.500548
5	1	-3.7905	-0.87246	-0.3316
6	1	-3.95209	-1.72874	1.196149
7	6	-2.97555	1.113571	0.896655
8	1	-3.47534	1.136344	-0.07119
9	1	-3.72011	1.394577	1.654565
10	1	-3.13384	-0.82219	3.038216
11	1	-1.97984	0.522958	3.009419
12	1	3.290793	2.665595	1.115495

13	6	2.316133	2.218426	0.876189
14	7	2.199343	0.827774	1.32175
15	1	1.541875	2.807623	1.36888
16	6	1.871149	0.705197	2.74578
17	6	3.393498	0.055355	0.946879
18	6	1.268657	-0.65161	3.064186
19	1	1.132913	1.472808	2.98197
20	1	2.75347	0.863102	3.386857
21	1	3.954349	0.611834	0.192835
22	1	4.069493	-0.07586	1.802584
23	8	0.105447	-0.82437	2.2493
24	1	0.987773	-0.68363	4.120688
25	1	1.970487	-1.4681	2.867019
26	1	-1.22656	-2.38432	2.46407
27	1	-0.91992	-1.44953	3.942999
28	6	-1.88754	2.196615	0.847391
29	6	-2.36483	-2.41711	-0.09234
30	6	2.0545	2.325718	-0.63057
31	6	3.09899	-1.31674	0.336057
32	8	1.577225	1.293258	-1.19933
33	8	2.284759	3.411918	-1.20303
34	8	4.080871	-2.01922	0.00379
35	8	1.884348	-1.63357	0.174956
36	8	-1.10735	-2.24205	-0.09468
37	8	-2.95542	-3.40572	-0.57703
38	8	-0.67537	1.820631	0.871549
39	8	-2.2874	3.37959	0.755915
40	8	0.074218	2.95822	-3.12214
41	8	-3.23108	2.68777	-2.01245
42	1	-0.34372	2.197139	-2.67679
43	1	0.888005	3.09096	-2.59425
44	1	-3.0943	3.155581	-1.16994
45	1	-2.56348	1.96243	-1.95486
46	8	2.84399	-2.41714	-2.65772
47	1	3.285076	-2.42798	-1.78681
48	1	1.975063	-1.9871	-2.46341
49	39	0.049953	-0.19945	-0.21951
50	9	0.471635	-1.23616	-2.18273
51	8	-1.24916	-3.14104	-3.02376
52	1	-1.77447	-3.3661	-2.23331
53	1	-0.62578	-2.44977	-2.6918
54	9	-1.36099	0.767807	-1.6514

Table S7. Optimized Cartesian coordinates (Å) of the $[F\subset[Y(OBETA)(H_2O)]_2]^{3-}\cdot 4H_2O$ system obtained with DFT calculations, fixing an Y-F distance of 2.33 Å.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.27071	2.064285	-2.05632
2	6	-4.56357	2.685931	-0.70368
3	7	-3.47046	2.539975	0.255928
4	6	-2.40918	3.517712	0.065226
5	1	-1.83349	3.606551	1.000802
6	1	-2.79996	4.524671	-0.18317
7	6	-3.97608	2.458336	1.620213
8	1	-3.18152	2.758424	2.316792
9	1	-4.83561	3.136186	1.79681
10	1	-4.83643	3.753767	-0.84106
11	1	-5.44665	2.168372	-0.29779
12	1	-4.58991	-3.76523	-0.09575
13	6	-4.23761	-2.73702	0.121517
14	7	-3.82716	-2.01658	-1.07921
15	1	-5.06665	-2.19112	0.597468
16	6	-4.95646	-1.46571	-1.82503
17	6	-2.93676	-2.82987	-1.90721
18	6	-4.57525	-0.27375	-2.68617
19	1	-5.70275	-1.11522	-1.09592
20	1	-5.44155	-2.2342	-2.46313
21	1	-2.41682	-3.55712	-1.26163
22	1	-3.50304	-3.42321	-2.65248
23	8	-3.98541	0.696392	-1.8447
24	1	-5.4928	0.13225	-3.14572
25	1	-3.877	-0.54344	-3.49672
26	1	-3.42042	2.546323	-2.56846
27	1	-5.16043	2.172899	-2.69972
28	6	-4.3642	1.02932	2.031515
29	6	-1.35592	3.117219	-0.97371
30	6	-3.11586	-2.77642	1.166373
31	6	-1.81832	-2.05274	-2.61605
32	8	-2.15413	-1.97877	0.988521
33	8	-3.23387	-3.55313	2.127504
34	8	-1.16694	-2.66628	-3.47738
35	8	-1.61695	-0.86961	-2.23357
36	8	-1.22545	1.859564	-1.1761
37	8	-0.67375	3.996411	-1.4952
38	8	-4.14876	0.107518	1.187953
39	8	-4.80394	0.861651	3.177356
40	8	-1.40112	1.066665	1.801468

41	1	-1.58324	0.628963	2.681879
42	1	-0.43005	1.249558	1.710375
43	8	-1.39567	-2.59318	3.960018
44	8	-2.17508	-0.05866	4.065086
45	1	-0.46667	-2.67441	3.631325
46	1	-1.98131	-2.98817	3.266611
47	1	-3.13493	0.006625	3.888615
48	1	-1.91299	-1.02737	4.022436
49	39	-2.26294	0.039442	-0.16445
50	9	-0.00974	-0.51921	0.035237
51	6	4.274579	1.902725	2.210063
52	6	4.519783	2.651339	0.913569
53	7	3.407382	2.564316	-0.03126
54	6	2.332634	3.50119	0.263396
55	1	1.720055	3.635268	-0.64356
56	1	2.71032	4.498009	0.566701
57	6	3.885154	2.619909	-1.40635
58	1	3.064562	2.951569	-2.05756
59	1	4.717099	3.340376	-1.53966
60	1	4.771245	3.709063	1.140168
61	1	5.404716	2.194733	0.443282
62	1	4.663398	-3.70702	-0.30336
63	6	4.287113	-2.66869	-0.40123
64	7	3.89681	-2.0862	0.87718
65	1	5.093258	-2.0606	-0.83856
66	6	5.027244	-1.57508	1.647478
67	6	3.045076	-2.99761	1.640702
68	6	4.631791	-0.47683	2.619916
69	1	5.750746	-1.14068	0.940699
70	1	5.545161	-2.38354	2.205731
71	1	2.562754	-3.70404	0.945516
72	1	3.638205	-3.61319	2.346318
73	8	4.009665	0.55444	1.879459
74	1	5.545015	-0.09335	3.106618
75	1	3.947642	-0.83776	3.406484
76	1	3.429713	2.317787	2.785888
77	1	5.179315	1.970714	2.837869
78	6	4.307535	1.247843	-1.95268
79	6	1.328229	3.002554	1.30736
80	6	3.136603	-2.62315	-1.41499
81	6	1.894113	-2.32541	2.401917
82	8	2.139297	-1.91311	-1.10424
83	8	3.266257	-3.25093	-2.47762
84	8	1.225537	-3.04492	3.161811
85	8	1.694477	-1.10406	2.166106
86	8	1.200761	1.730797	1.389368

87	8	0.674674	3.825976	1.944365
88	8	4.091784	0.240434	-1.21432
89	8	4.768257	1.208056	-3.10237
90	8	1.336451	1.195328	-1.65172
91	1	1.533277	0.920259	-2.59036
92	1	0.367867	1.387453	-1.54713
93	8	1.438748	-2.0954	-4.20811
94	8	2.127887	0.45818	-4.07609
95	1	0.506028	-2.22599	-3.90574
96	1	2.019808	-2.5595	-3.55491
97	1	3.09126	0.532034	-3.92356
98	1	1.901985	-0.51753	-4.15104
99	39	2.250398	0.025161	0.191304

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