Electronic Supporting Information (ESI)

Effect of Hydration Equilibria on the Relaxometric Properties of Gd(III) Complexes: New Insights into Old Systems

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Content

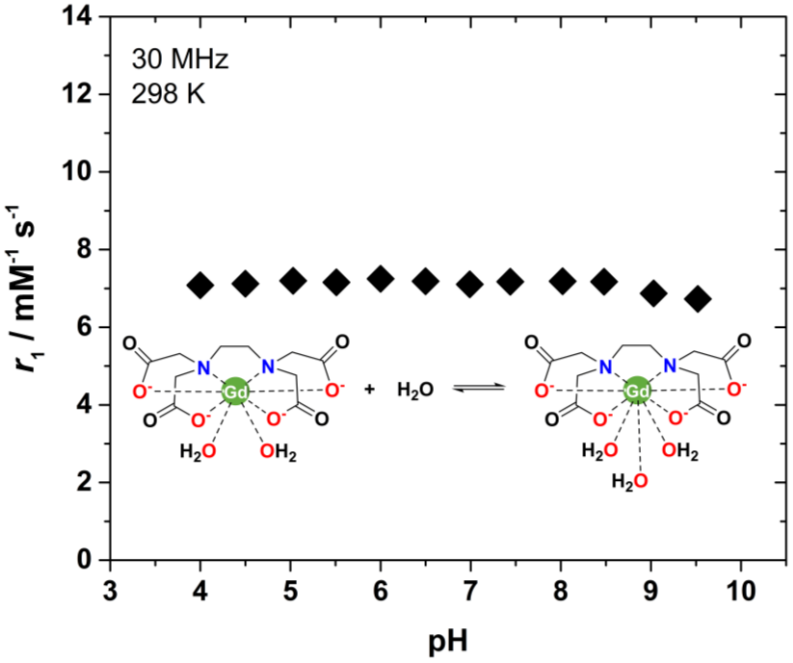

Figure S1: pH dependency of r_1 of $[Gd(EDTA)(H_2O)_q]^-$ (30 MHz, 298K). Relaxivity values are constant between pH 4 and 8.5.

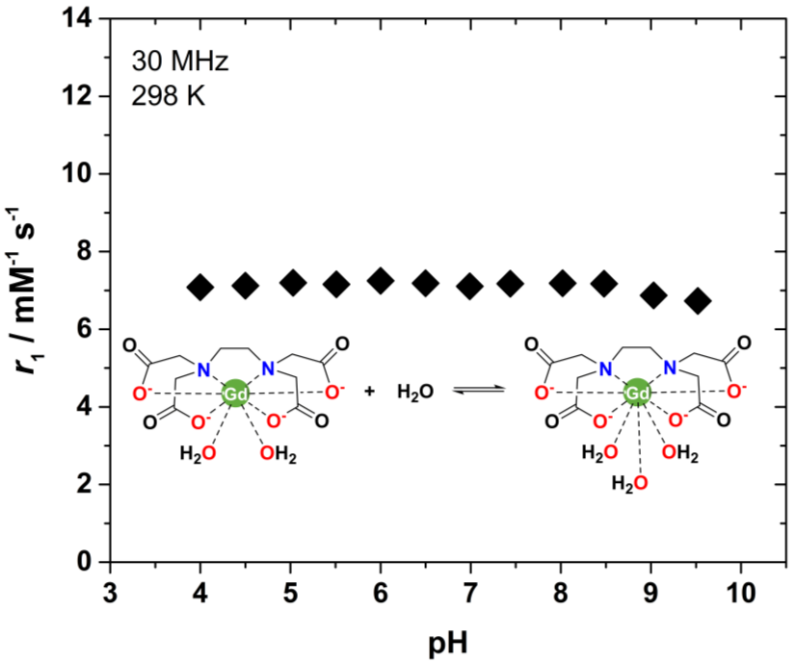

Figure S2: pH dependency of r_1 of $[Gd(CDTA)(H_2O)_q]^-$ (30 MHz, 298K). Relaxivity values are constant throughout the investigated pH range.

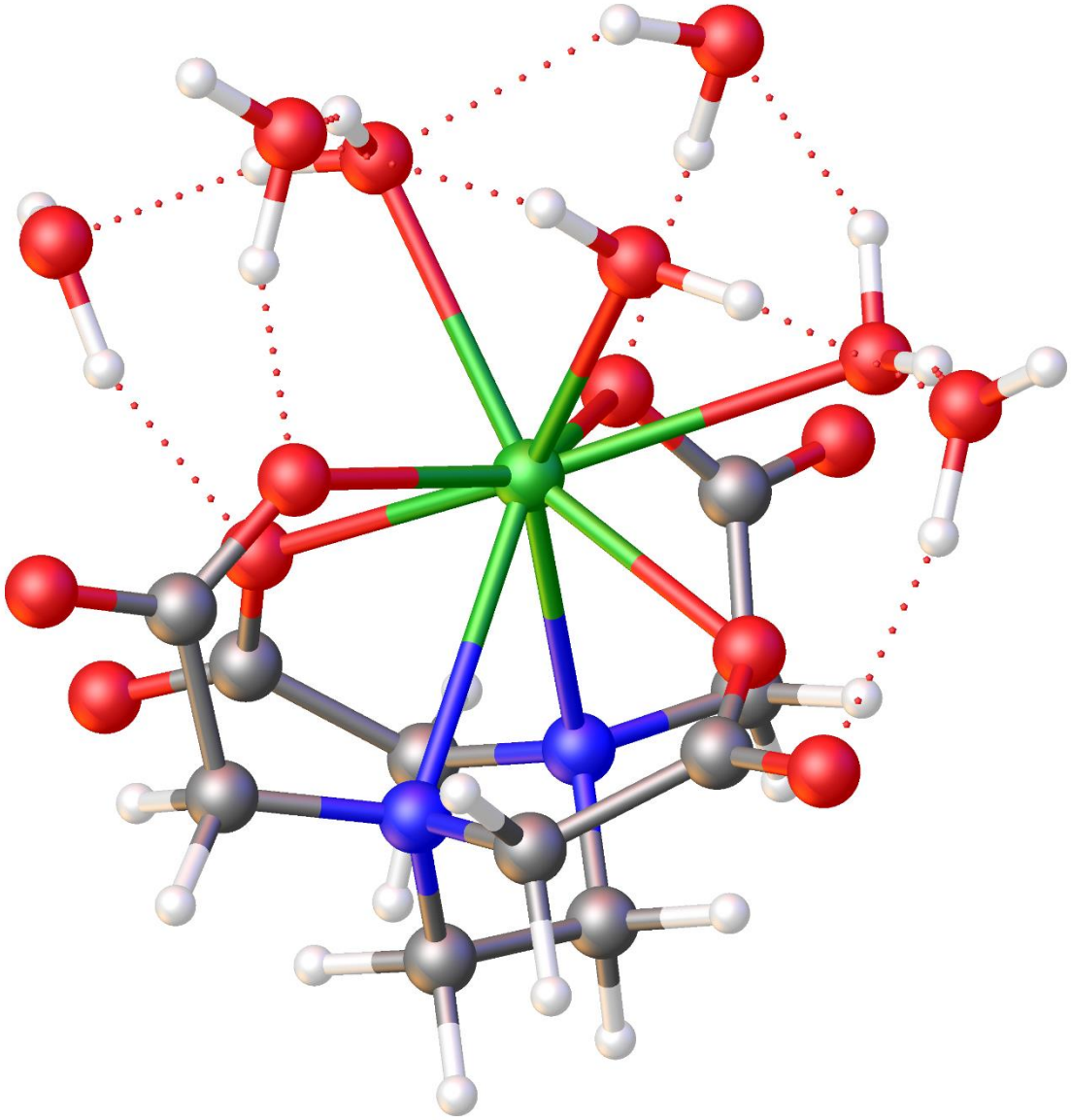

Figure S3: Structure of the $[Gd(EDTA)(H_2O)_3]^{3+}\cdot 4H_2O$ system obtained with DFT calculations (wB97XD/LCECP/Def2-TZVPP).

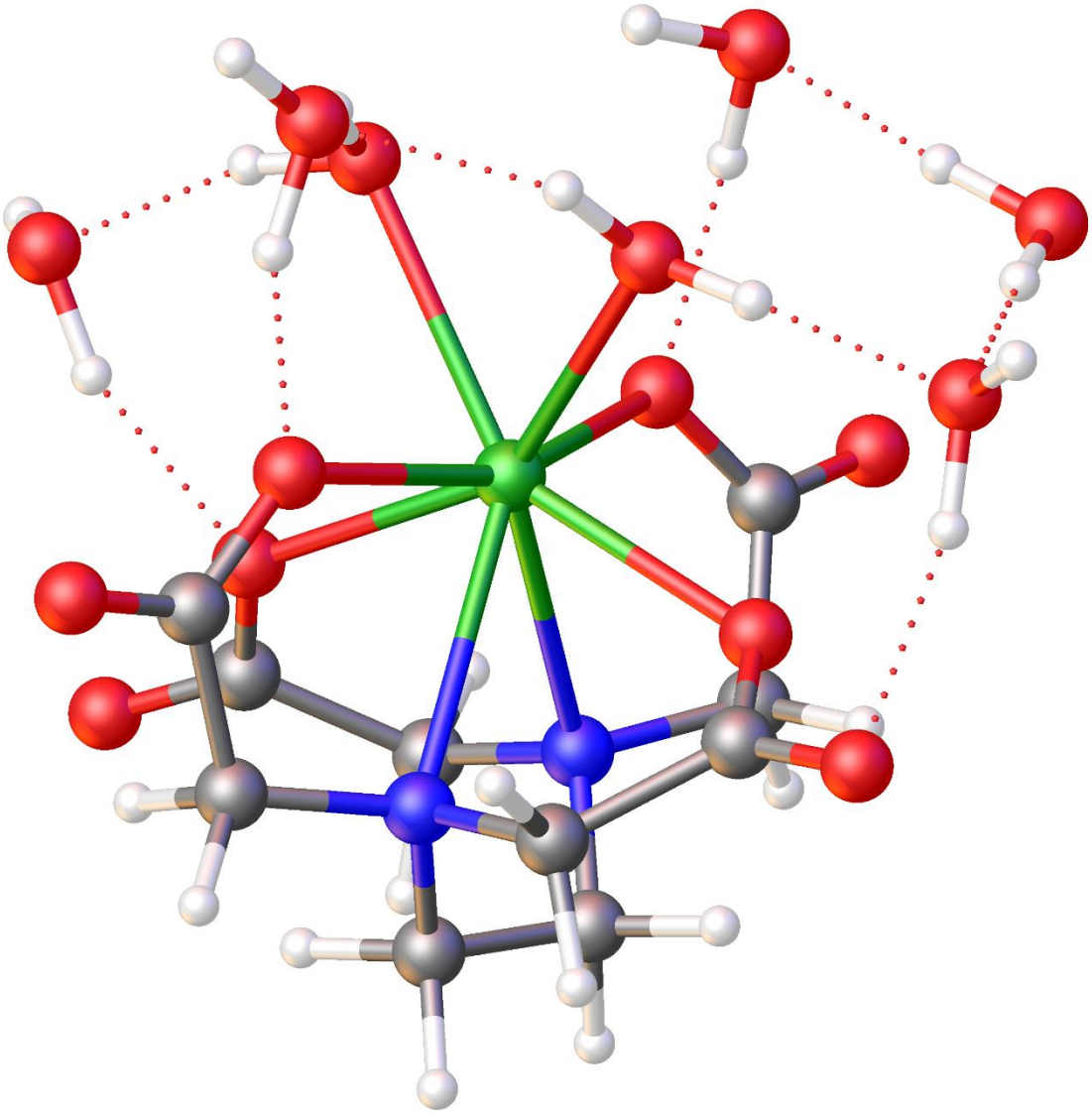

Figure S4: Structure of the $[Gd(EDTA)(H_2O)_2]^{3+}\cdot 5H_2O$ system obtained with DFT calculations (wB97XD/LCECP/Def2-TZVPP).

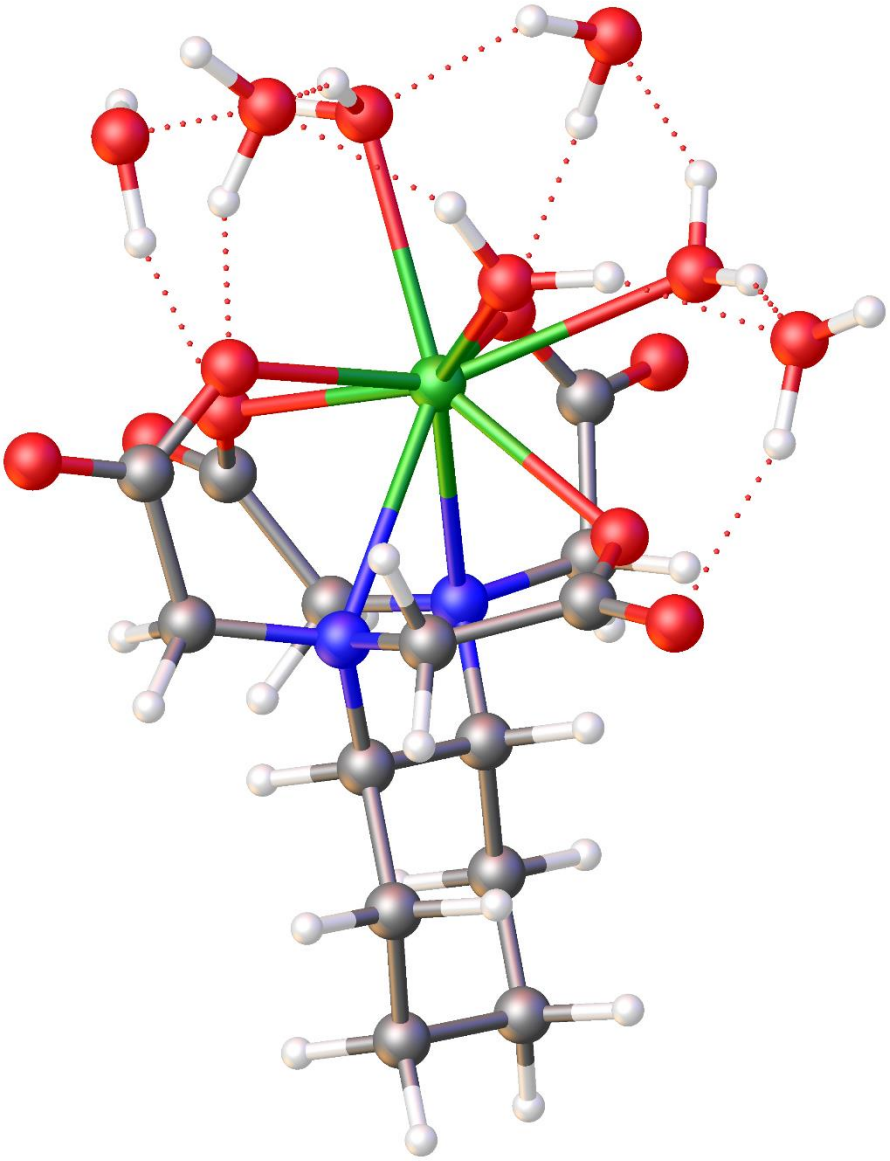

Figure S5: Structure of the $[Gd(CDTA)(H_2O)_3]^{3+}\cdot 4H_2O$ system obtained with DFT calculations (wB97XD/LCECP/Def2-TZVPP).

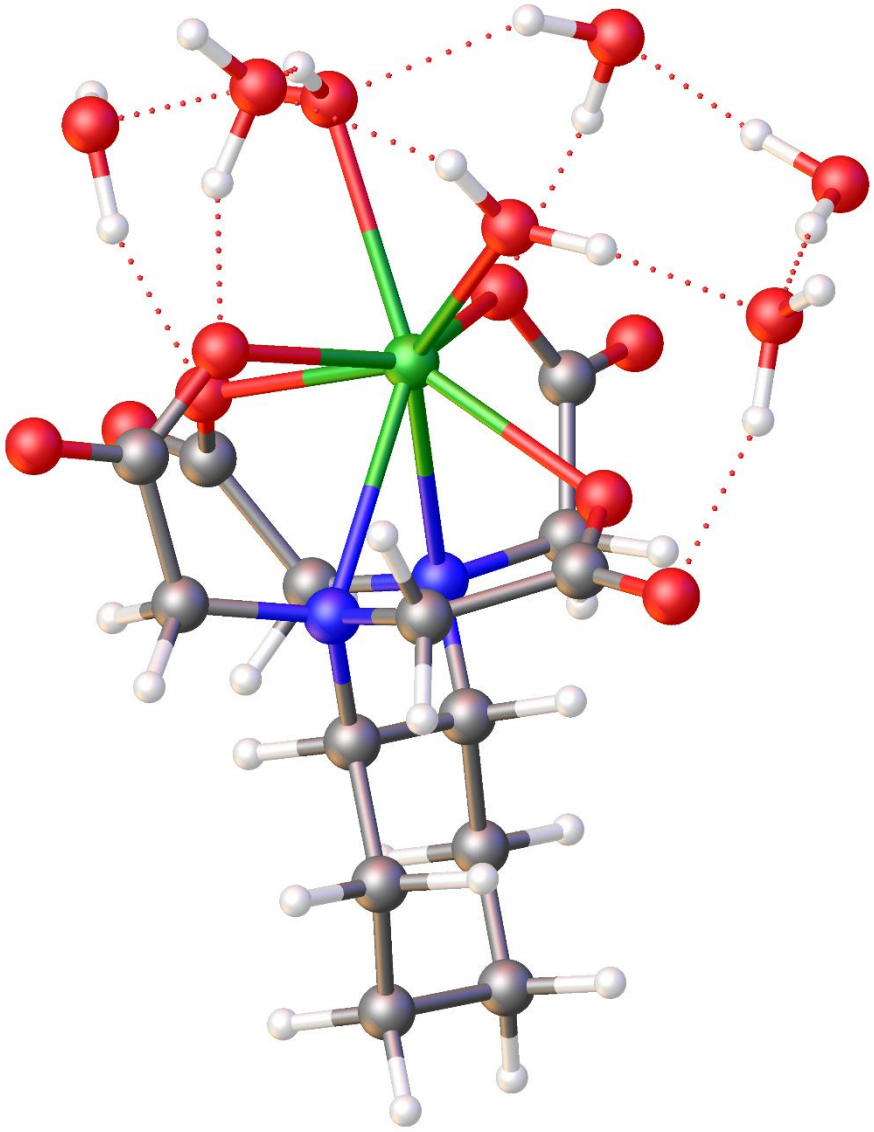

Figure S5: Structure of the $[Gd(CDTA)(H_2O)_2]^{3+}\cdot 5H_2O$ system obtained with DFT calculations (wB97XD/LCECP/Def2-TZVPP).

Table S1: Cartesian coordinates obtained with DFT calculations for the $[Gd(H_2O)_8]^{3+}\cdot 19H_2O$ system (wB97XD/LCECP/Def2-TZVPP, 0 imaginary frequencies).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	-0.027286	0.222621	0.496264
2	8	0	2.002585	-0.053248	1.816816
3	1	0	2.019011	-0.059397	2.789102
4	1	0	2.763205	-0.578429	1.487191
5	8	0	-0.058028	2.032645	2.144948
6	1	0	0.718526	2.383539	2.617328
7	1	0	-0.835231	2.233941	2.692730
8	8	0	1.452116	-1.063043	-0.901019
9	1	0	1.460965	-1.996155	-1.177519

10	1	0	2.287829	-0.664365	-1.221971
11	8	0	-0.135659	-2.064693	1.579356
12	1	0	0.641832	-2.652653	1.485128
13	1	0	-0.930630	-2.586679	1.356110
14	8	0	1.615156	1.807495	-0.338643
15	1	0	1.667706	2.293493	-1.181177
16	1	0	2.346445	2.121327	0.238243
17	8	0	-0.641893	0.466499	-3.657043
18	1	0	0.222829	0.277298	-4.042057
19	1	0	-1.329444	-0.025206	-4.122943
20	8	0	-2.104714	0.173959	1.862398
21	1	0	-1.926282	-0.172473	2.750296
22	1	0	-2.914212	-0.275069	1.525095
23	8	0	-1.498565	-1.214503	-0.832875
24	1	0	-1.252524	-1.939994	-1.427742
25	1	0	-2.305358	-0.814323	-1.212745
26	8	0	-1.661624	1.794309	-0.532205
27	1	0	-1.417282	2.329287	-1.314328
28	1	0	-2.175351	2.381537	0.072677
29	8	0	3.991878	-1.628676	0.875668
30	8	0	2.031965	-3.647888	1.078504
31	8	0	1.665939	0.164049	4.535230
32	8	0	-0.795169	-0.990765	4.064183
33	8	0	-3.121916	3.384358	1.035846
34	8	0	-3.692868	0.100491	-1.704347
35	8	0	3.768375	-0.148237	-1.922059
36	8	0	2.198460	0.678555	-4.065724
37	8	0	1.460168	-3.732246	-1.569006
38	8	0	-1.028545	-3.337661	-2.610951
39	8	0	-4.197320	-1.149821	0.832203
40	8	0	1.685891	3.059802	-2.777382
41	8	0	-0.993545	2.951169	-2.898342
42	8	0	3.596612	2.690815	1.262720
43	8	0	2.138342	2.692561	3.631776
44	1	0	-4.242389	-0.837406	-0.081271
45	1	0	-3.212244	0.908826	-1.482451
46	1	0	-4.058132	3.221460	0.915626
47	1	0	-3.738561	-2.002479	0.800159
48	1	0	-3.646803	-0.004983	-2.669007
49	1	0	-2.939563	3.204380	1.972156
50	1	0	3.197962	2.683573	2.149405
51	1	0	4.291974	2.032535	1.292585
52	1	0	3.359523	0.090794	-2.775296
53	1	0	4.061742	0.682408	-1.544151
54	1	0	3.447328	-2.432607	0.891458
55	1	0	4.144373	-1.433687	-0.053071
56	1	0	2.082741	1.593734	-3.748192
57	1	0	1.836194	-3.919061	0.163231
58	1	0	2.058164	1.881189	4.164104
59	1	0	2.135099	3.435027	4.236497
60	1	0	2.569151	0.745185	-4.946690
61	1	0	2.172146	-4.447391	1.587306
62	1	0	0.739355	3.270688	-2.898672
63	1	0	0.584964	-3.805017	-1.989029
64	1	0	0.759656	-0.197298	4.548980
65	1	0	2.181602	3.871452	-2.888545
66	1	0	2.179652	-0.345779	5.162334
67	1	0	2.107206	-4.018393	-2.214839
68	1	0	-0.960781	2.066602	-3.335951
69	1	0	-1.210593	-1.533600	4.735904

70	1	0	-1.728620	-3.993050	-2.584223
71	1	0	-1.615630	3.496751	-3.379811
72	1	0	-0.496647	-1.593623	3.361396
73	1	0	-0.980636	-3.040016	-3.521893
74	1	0	-2.751636	-3.955749	1.937111
75	1	0	-2.489399	-4.063108	0.435698
76	1	0	-2.774439	2.058507	4.053548
77	1	0	-2.175728	3.452586	4.282184
78	1	0	-3.605061	0.034219	-5.101566
79	1	0	-3.410437	-1.396012	-4.600781
80	8	0	-2.285134	2.762901	3.625046
81	8	0	-3.193370	-0.482411	-4.406416
82	8	0	-2.505116	-3.441212	1.165686

[a] E(RwB97XD) = -2100.1739537; Zero-point correction = 0.695268 Hartree; Thermal correction to Energy = 0.763957; Thermal correction to Enthalpy = 0.764901; Thermal correction to Gibbs Free Energy = 0.593869; Sum of electronic and zero-point Energies = -2099.478686; Sum of electronic and thermal Energies = -2099.409997; Sum of electronic and thermal Enthalpies = -2099.409053; Sum of electronic and thermal Free Energies = -2099.580084.

Table S2: Cartesian coordinates obtained with DFT calculations for the $[Gd(H_2O)_9]^{3+}\cdot 18H_2O$ system (wB97XD/LCECP/Def2-TZVPP, 0 imaginary frequencies).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	0.179450	0.120792	0.063107
2	8	0	2.164861	-0.120028	1.530944
3	1	0	2.013842	-0.140930	2.490739
4	1	0	2.814088	-0.826584	1.334422
5	8	0	0.156336	1.910148	1.785465
6	1	0	0.858876	2.269385	2.351258
7	1	0	-0.688761	2.277049	2.088300
8	8	0	1.784213	-1.330134	-1.084712
9	1	0	1.624880	-2.218172	-1.443980
10	1	0	2.549461	-0.938733	-1.555418
11	8	0	0.058903	-2.149213	1.105431
12	1	0	0.730374	-2.851024	1.073794
13	1	0	-0.803768	-2.559884	1.267913
14	8	0	1.918302	1.717276	-0.621791
15	1	0	1.761051	2.429730	-1.264708
16	1	0	2.554753	2.052435	0.044345
17	8	0	0.074107	0.674663	-2.416940
18	1	0	0.828131	0.746713	-3.022403
19	1	0	-0.689338	0.388670	-2.939585
20	8	0	-1.744171	-0.034447	1.657749
21	1	0	-1.590886	-0.192294	2.602269
22	1	0	-2.572206	-0.470586	1.400257
23	8	0	-1.581007	-1.220156	-1.015171
24	1	0	-1.571311	-2.132878	-1.341425
25	1	0	-2.406210	-0.800311	-1.308801
26	8	0	-1.602940	1.701916	-0.554428
27	1	0	-1.557381	2.334824	-1.287317
28	1	0	-2.446915	1.816717	-0.080668
29	8	0	3.967286	-2.127425	1.117099
30	8	0	2.011563	-4.070296	0.752091
31	8	0	1.615870	0.043536	4.244302
32	8	0	-1.123537	-0.419143	4.358560

33	8	0	-4.008999	1.877511	0.778439
34	8	0	-3.970899	-0.064948	-1.856247
35	8	0	3.886611	-0.098755	-2.273979
36	8	0	2.269588	1.379767	-3.968903
37	8	0	1.259488	-3.930744	-1.852202
38	8	0	-1.483355	-3.793114	-2.103363
39	8	0	-4.186164	-1.144047	0.850530
40	8	0	1.414367	3.576214	-2.604136
41	8	0	-1.361355	3.600094	-2.609209
42	8	0	3.747186	2.649111	1.171140
43	8	0	2.210487	2.587220	3.488677
44	1	0	-4.245986	-1.094223	-0.110392
45	1	0	-4.033898	0.837233	-1.534090
46	1	0	-4.220942	0.981716	1.061108
47	1	0	-3.801850	-2.011435	1.049731
48	1	0	-3.558614	0.000623	-2.733185
49	1	0	-3.559293	2.283158	1.537104
50	1	0	3.296862	2.627474	2.032325
51	1	0	4.407046	1.956296	1.221535
52	1	0	3.420071	0.438488	-2.937825
53	1	0	4.098468	0.524864	-1.576758
54	1	0	3.363906	-2.873424	0.956896
55	1	0	4.422934	-1.990142	0.285794
56	1	0	2.087907	2.293216	-3.684527
57	1	0	1.807647	-4.247500	-0.184341
58	1	0	2.098946	1.752747	3.978559
59	1	0	2.163348	3.302914	4.122543
60	1	0	2.289243	1.375597	-4.925871
61	1	0	2.019176	-4.911818	1.208510
62	1	0	0.444256	3.657222	-2.645971
63	1	0	0.300080	-3.994500	-2.006562
64	1	0	0.664048	-0.127817	4.359528
65	1	0	1.768872	4.464903	-2.565278
66	1	0	2.077361	-0.511623	4.873436
67	1	0	1.694428	-4.330841	-2.605648
68	1	0	-1.718543	3.302628	-3.448233
69	1	0	-1.596167	0.180102	4.940120
70	1	0	-1.987616	-4.482179	-1.666265
71	1	0	-1.792111	4.437299	-2.424458
72	1	0	-1.338588	-1.301837	4.667823
73	1	0	-1.806863	-3.767259	-3.006482
74	1	0	-2.571592	-3.352116	2.634334
75	1	0	-2.618722	-4.163670	1.344477
76	1	0	-2.442293	2.876255	3.600492
77	1	0	-2.255726	4.023493	2.610041
78	1	0	-2.305464	0.526101	-4.760481
79	1	0	-2.087766	-0.939106	-4.385642
80	8	0	-2.278392	3.066608	2.674846
81	8	0	-2.190627	-0.061733	-4.011145
82	8	0	-2.498109	-3.273478	1.680797

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[a] E(RwB97XD) = -2100.1677143 ; Zero-point correction = 0.692793 Hartree; Thermal correction to Energy = 0.763807; Thermal correction to Enthalpy = 0.764751; Thermal correction to Gibbs Free Energy = 0.589295; Sum of electronic and zero-point Energies = -2099.474921; Sum of electronic and thermal Energies = -2099.403907; Sum of electronic and thermal Enthalpies = -2099.402963; Sum of electronic and thermal Free Energies = -2099.578419.

Table S3: Cartesian coordinates obtained with DFT calculations for the transition state responsible for the $[Gd(H_2O)_9]^{3+}\cdot 18H_2O \leftrightarrow [Gd(H_2O)_8]^{3+}\cdot 19H_2O$ interconversion (wB97XD/LCECP/Def2-TZVPP, 1 imaginary frequency).[a]

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
Gd	-0.07395910	0.17792057	0.37343719	
O	1.97352872	-0.05103452	1.67597338	
H	1.99070132	-0.02244538	2.64817963	
H	2.72573709	-0.60353577	1.37143393	
O	-0.06672938	1.99171009	2.02698649	
H	0.71129886	2.36241922	2.48103989	
H	-0.83147150	2.18858024	2.59341123	
O	1.40244240	-1.14668309	-0.98721566	
H	1.42358358	-2.09243616	-1.21561395	
H	2.25283353	-0.76113216	-1.28393507	
O	-0.16472101	-2.07093502	1.54225319	
H	0.61143954	-2.66401605	1.47368159	
H	-0.95880750	-2.60179213	1.33747312	
O	1.53419592	1.74844239	-0.53215865	
H	1.57208490	2.28624609	-1.34314683	
H	2.23828115	2.09001714	0.06473558	
O	-0.39117912	0.54896328	-3.02104439	
H	0.46263500	0.37602165	-3.44541029	
H	-1.06595145	0.02156814	-3.47012896	
O	-2.12996317	0.15294745	1.77526482	
H	-1.93010122	-0.15165124	2.67422608	
H	-2.94569233	-0.31543130	1.48285365	
O	-1.57567022	-1.29450586	-0.85781540	
H	-1.33163072	-2.00511352	-1.47326763	
H	-2.40642259	-0.90375606	-1.19224158	
O	-1.73453410	1.79857986	-0.54395972	
H	-1.50106866	2.39606181	-1.27946972	
H	-2.24899114	2.33677799	0.10643262	
O	3.94926652	-1.69379513	0.83560468	
O	1.98895516	-3.69105978	1.11076239	
O	1.67261087	0.21689714	4.39892980	
O	-0.80799083	-0.92271350	4.00061013	
O	-3.22668380	3.27908451	1.09128795	
O	-3.76503162	0.09572801	-1.63536660	
O	3.77482446	-0.22136793	-1.89835595	
O	2.25244946	0.77585056	-3.96605692	
O	1.41668530	-3.84576206	-1.52916905	
O	-1.04765429	-3.40228297	-2.61632121	
O	-4.24753812	-1.22095091	0.87209781	
O	1.68573275	3.21805118	-2.85333569	
O	-1.00917428	3.10922573	-2.85429761	
O	3.44984836	2.78024103	1.06297577	
O	2.11447576	2.74200364	3.49219586	
H	-4.32881870	-0.91742271	-0.04127074	
H	-3.25619862	0.87707570	-1.37400460	
H	-4.14774818	3.02947485	1.00790742	
H	-3.78569701	-2.07181767	0.83380425	
H	-3.64731036	0.01050354	-2.59511853	
H	-2.99185229	3.11745918	2.01914008	
H	3.09149832	2.77019627	1.96655795	
H	4.22999904	2.22547804	1.09504697	
H	3.38408802	0.09293794	-2.73541897	
H	4.06104102	0.57561756	-1.44952143	

H	3.40592066	-2.49710894	0.88662354
H	4.11421073	-1.54596645	-0.09969629
H	2.16696195	1.72313761	-3.75427092
H	1.79066564	-3.98807722	0.20402928
H	2.05388697	1.93395106	4.03214530
H	2.07717110	3.49152462	4.08687049
H	2.47478647	0.71860013	-4.89593963
H	2.11686945	-4.47540298	1.64569935
H	0.75196157	3.47416843	-2.96584117
H	0.54019267	-3.91360395	-1.94664647
H	0.76290499	-0.13403005	4.43595983
H	2.20945916	4.01961188	-2.84187085
H	2.19504036	-0.29554510	5.01667695
H	2.05719708	-4.16424409	-2.16636336
H	-0.87415345	2.17965079	-3.14505118
H	-1.22333757	-1.43413088	4.69668101
H	-1.76082130	-4.04418768	-2.60945754
H	-1.66939560	3.50216955	-3.42573177
H	-0.52149211	-1.55534715	3.31944561
H	-0.93987831	-3.13783509	-3.53242133
H	-2.74486697	-4.01390771	1.94332063
H	-2.50141578	-4.10448477	0.43738090
H	-2.65600474	2.06439446	4.14615010
H	-2.03186540	3.46249878	4.23114925
H	-2.99576468	0.29669388	-4.91864806
H	-3.02508059	-1.19726881	-4.59935432
O	-2.20913601	2.73704156	3.62956090
O	-2.81374455	-0.34020777	-4.22502139
O	-2.52160950	-3.48837099	1.17225479

[a] E(RwB97XD) = -2100.1705257 Hartree; Zero-point correction = 0.695785; Thermal correction to Energy = 0.763732; Thermal correction to Enthalpy = 0.764676; Thermal correction to Gibbs Free Energy = 0.595320; Sum of electronic and zero-point Energies = -2099.474741; Sum of electronic and thermal Energies = -2099.406794; Sum of electronic and thermal Enthalpies = -2099.405850; Sum of electronic and thermal Free Energies = -2099.575206.

Table S4: Cartesian coordinates obtained with DFT calculations for the $[Gd(EDTA)(H_2O)_3]^{-}\cdot 4H_2O$ system (wB97XD/LCECP/Def2-TZVPP, 0 imaginary frequencies).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	2.946486	7.277871	2.400948
2	8	0	4.550157	5.996373	3.515464
3	8	0	1.250244	7.246279	4.122287
4	8	0	0.975684	6.707582	1.177268
5	8	0	3.592628	7.892131	0.127430
6	8	0	5.091301	5.129611	5.475728
7	8	0	-0.585850	6.435000	5.078152
8	8	0	-0.125178	5.669103	-0.449563
9	8	0	5.197414	7.529000	-1.376775
10	6	0	4.316851	5.264279	4.522450
11	6	0	2.960925	4.568135	4.565004
12	1	0	3.113018	3.501044	4.754350
13	1	0	2.454240	4.968446	5.443352
14	6	0	0.723875	4.946568	3.766119
15	1	0	0.387014	4.156847	4.443862
16	1	0	0.105726	4.897828	2.869943

17	6	0	0.423125	6.307336	4.394250
18	6	0	4.447085	7.158642	-0.480202
19	6	0	4.537650	5.704825	0.004540
20	1	0	4.785432	5.054044	-0.838954
21	1	0	5.367040	5.662735	0.714089
22	6	0	2.189604	5.217824	-0.256031
23	1	0	1.965213	4.183199	-0.523465
24	1	0	2.465381	5.716897	-1.185154
25	6	0	0.896492	5.899392	0.188281
26	6	0	2.307114	3.766444	2.349874
27	1	0	1.394867	3.721088	1.756399
28	1	0	2.429798	2.776561	2.801810
29	6	0	3.483686	4.032237	1.425615
30	1	0	4.407012	4.098661	1.995840
31	1	0	3.580183	3.187045	0.733786
32	7	0	3.312772	5.291252	0.689231
33	7	0	2.125836	4.798820	3.381058
34	8	0	5.469152	8.127420	2.176209
35	1	0	5.411165	9.060801	1.925033
36	1	0	5.878005	8.074632	3.049560
37	8	0	1.844116	9.581938	2.208404
38	1	0	1.009526	9.533004	1.695631
39	1	0	1.589233	9.890954	3.094854
40	8	0	3.714314	8.826341	4.291320
41	1	0	4.508387	8.550229	4.781036
42	1	0	3.072602	9.218487	4.895350
43	8	0	6.119856	7.778171	5.067447
44	8	0	4.391986	10.432158	0.862877
45	8	0	1.221091	9.756556	4.909789
46	8	0	-0.478655	8.970406	0.969582
47	1	0	0.538290	10.162160	5.441719
48	1	0	0.990958	8.808090	4.784462
49	1	0	5.923506	6.835656	5.226799
50	1	0	6.707957	8.065633	5.765313
51	1	0	3.614717	10.553410	1.419230
52	1	0	4.148931	9.640025	0.349994
53	1	0	-0.613539	9.188143	0.047116
54	1	0	-0.131927	8.053881	0.979550

E(RwB97XD) = -1671.3904055 Hartree; Zero-point correction = 0.420577; Thermal correction to Energy = 0.457480; Thermal correction to Enthalpy = 0.458424; Thermal correction to Gibbs Free Energy = 0.353910; Sum of electronic and zero-point Energies = -1670.969828; Sum of electronic and thermal Energies = -1670.932926; Sum of electronic and thermal Enthalpies = -1670.931981; Sum of electronic and thermal Free Energies = -1671.036495.

Table S5: Cartesian coordinates obtained with DFT calculations for the $[Gd(EDTA)(H_2O)_2]^{-}\cdot 5H_2O$ system (wB97XD/LCECP/Def2-TZVPP, 0 imaginary frequencies).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	2.719263	7.225956	2.345499
2	8	0	4.503552	6.072293	3.289898
3	8	0	1.128186	7.248233	4.145365
4	8	0	0.831480	6.600445	1.086453
5	8	0	3.790529	7.834153	0.293061
6	8	0	5.236365	5.121748	5.150989
7	8	0	-0.455047	6.339141	5.417519

8	8	0	-0.208356	5.503631	-0.542930
9	8	0	5.350088	7.406902	-1.239279
10	6	0	4.374748	5.293401	4.283765
11	6	0	3.030248	4.586200	4.450288
12	1	0	3.207238	3.519496	4.614614
13	1	0	2.616045	4.977121	5.380096
14	6	0	0.704909	4.918077	3.902062
15	1	0	0.469880	4.108615	4.597693
16	1	0	0.000989	4.856440	3.071245
17	6	0	0.425960	6.263737	4.571859
18	6	0	4.561289	7.053232	-0.374452
19	6	0	4.489834	5.573373	0.013296
20	1	0	4.705625	4.955367	-0.862421
21	1	0	5.287741	5.410363	0.740171
22	6	0	2.135848	5.201199	-0.356090
23	1	0	1.970877	4.191030	-0.737811
24	1	0	2.429770	5.812447	-1.210785
25	6	0	0.797271	5.787290	0.092518
26	6	0	2.136974	3.774936	2.325362
27	1	0	1.207409	3.803719	1.758556
28	1	0	2.197849	2.778548	2.775769
29	6	0	3.305780	3.960990	1.378991
30	1	0	4.241706	3.960952	1.932582
31	1	0	3.336444	3.110251	0.688982
32	7	0	3.214127	5.228320	0.641162
33	7	0	2.064528	4.814960	3.364997
34	8	0	6.646744	9.053943	2.528326
35	1	0	5.842396	9.486792	2.205687
36	1	0	6.414216	8.639196	3.366517
37	8	0	1.668658	9.527813	2.120237
38	1	0	0.826460	9.479346	1.619919
39	1	0	1.441295	9.872490	3.001089
40	8	0	3.720750	8.810717	4.043587
41	1	0	4.478655	8.498762	4.573015
42	1	0	3.108643	9.293853	4.615254
43	8	0	6.018752	7.808856	5.132800
44	8	0	4.487605	10.345651	1.115904
45	8	0	1.293910	9.791578	4.839563
46	8	0	-0.648693	8.875400	0.889193
47	1	0	0.728141	10.257073	5.453571
48	1	0	1.006660	8.853299	4.802499
49	1	0	5.897563	6.839038	5.155162
50	1	0	6.392592	8.063427	5.976116
51	1	0	3.678236	10.497449	1.611565
52	1	0	4.296275	9.520853	0.633429
53	1	0	-0.797223	9.103973	-0.028607
54	1	0	-0.308291	7.959120	0.884413

E(RwB97XD) = -1671.3922758 Hartree; Zero-point correction = 0.419738; Thermal correction to Energy = 0.457083; Thermal correction to Enthalpy = 0.458027; Thermal correction to Gibbs Free Energy = 0.351942; Sum of electronic and zero-point Energies = -1670.972538; Sum of electronic and thermal Energies = -1670.935193; Sum of electronic and thermal Enthalpies = -1670.934249; Sum of electronic and thermal Free Energies = -1671.040334.

Table S6: Cartesian coordinates obtained with DFT calculations for the transition state responsible for the $[Gd(EDTA)(H_2O)_2]^-\cdot 5H_2O \leftrightarrow [Gd(EDTA)(H_2O)_3]^-\cdot 4H_2O$ interconversion (wB97XD/LCECP/Def2-TZVPP, 1 imaginary frequency).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	2.845674	7.251935	2.381061
2	8	0	4.518770	6.051627	3.458179
3	8	0	1.197050	7.252230	4.132322
4	8	0	0.919615	6.657422	1.139560
5	8	0	3.669966	7.894100	0.220103
6	8	0	5.121402	5.150056	5.386686
7	8	0	-0.542794	6.389739	5.217027
8	8	0	-0.152422	5.573424	-0.476835
9	8	0	5.219076	7.523300	-1.338416
10	6	0	4.321890	5.295553	4.456430
11	6	0	2.975370	4.582352	4.528014
12	1	0	3.144636	3.515720	4.701931
13	1	0	2.490138	4.968038	5.424880
14	6	0	0.707842	4.941975	3.802734
15	1	0	0.401468	4.137062	4.476132
16	1	0	0.064849	4.902692	2.923220
17	6	0	0.415897	6.290516	4.462290
18	6	0	4.481558	7.149084	-0.435673
19	6	0	4.529305	5.680483	0.005077
20	1	0	4.768946	5.046153	-0.852512
21	1	0	5.348826	5.600623	0.722716
22	6	0	2.181818	5.213001	-0.297175
23	1	0	1.992792	4.184956	-0.613569
24	1	0	2.459053	5.763960	-1.196547
25	6	0	0.863258	5.840579	0.152562
26	6	0	2.253479	3.778337	2.335517
27	1	0	1.338397	3.756507	1.745255
28	1	0	2.353737	2.785896	2.786898
29	6	0	3.434681	4.020749	1.412013
30	1	0	4.358059	4.074248	1.983916
31	1	0	3.520123	3.170874	0.725072
32	7	0	3.287215	5.279634	0.669132
33	7	0	2.100358	4.813339	3.370820
34	8	0	5.975871	8.274178	2.173882
35	1	0	5.562165	9.139069	2.056232
36	1	0	6.092052	8.146841	3.122042
37	8	0	1.741468	9.549911	2.165491
38	1	0	0.905938	9.496918	1.654412
39	1	0	1.496873	9.878355	3.047776
40	8	0	3.764042	8.850037	4.126822
41	1	0	4.522169	8.542682	4.657627
42	1	0	3.128341	9.298650	4.700739
43	8	0	6.072034	7.792182	5.129970
44	8	0	4.370512	10.429249	1.041199
45	8	0	1.305223	9.778266	4.880312
46	8	0	-0.568528	8.910378	0.920989
47	1	0	0.710432	10.221396	5.483286
48	1	0	1.032850	8.836721	4.810037
49	1	0	5.890251	6.840509	5.257781
50	1	0	6.575693	8.088810	5.887397
51	1	0	3.562937	10.505439	1.560196
52	1	0	4.194320	9.629419	0.514738
53	1	0	-0.704092	9.129318	-0.001145
54	1	0	-0.218091	7.996706	0.929658

E(RwB97XD) = =-1671.3885565 Hartree; Zero-point correction = 0.420425; Thermal correction to Energy = 0.456627; Thermal correction to Enthalpy = 0.457571; Thermal correction to Gibbs Free Energy =

0.354951; Sum of electronic and zero-point Energies = -1670.968132; Sum of electronic and thermal Energies = -1670.931930; Sum of electronic and thermal Enthalpies = -1670.930985; Sum of electronic and thermal Free Energies = -1671.033606.

Table S7: Cartesian coordinates obtained with DFT calculations for the $[Gd(CDTA)(H_2O)_3]^{-}\cdot 4H_2O$ system (wB97XD/LCECP/Def2-TZVPP, 0 imaginary frequencies).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	2.842334	7.202388	2.414553
2	8	0	4.513486	5.798152	3.356958
3	8	0	0.943161	7.343611	3.910009
4	8	0	0.881869	6.945375	1.059069
5	8	0	3.478652	7.854638	0.166434
6	8	0	5.016868	5.004478	5.362901
7	8	0	-0.860702	6.488184	4.888730
8	8	0	0.225129	6.667890	-1.046946
9	8	0	4.876658	7.396836	-1.505075
10	6	0	4.221641	5.205456	4.437821
11	6	0	2.756075	4.822440	4.622417
12	1	0	2.675785	3.880250	5.164069
13	1	0	2.354865	5.593073	5.283675
14	6	0	0.549923	4.998310	3.693832
15	1	0	0.201703	4.239927	4.400660
16	1	0	-0.021418	4.881803	2.772589
17	6	0	0.167969	6.379705	4.229603
18	6	0	4.198642	7.068070	-0.536906
19	6	0	4.238940	5.606533	-0.076062
20	1	0	4.416883	4.976695	-0.950350
21	1	0	5.107429	5.515215	0.581124
22	6	0	1.868476	5.177306	-0.206119
23	1	0	1.243129	4.315987	0.027379
24	1	0	2.159757	5.066126	-1.251249
25	6	0	0.926134	6.373123	-0.084558
26	6	0	2.189660	3.687216	2.464903
27	1	0	1.244353	3.568015	1.933287
28	6	0	3.272349	3.924263	1.399177
29	1	0	4.225422	4.046096	1.910337
30	7	0	3.046233	5.201559	0.675960
31	7	0	1.974892	4.853911	3.376461
32	8	0	5.205739	8.206401	2.321725
33	1	0	5.254987	9.102425	1.955385
34	1	0	5.716534	8.151277	3.140497
35	8	0	2.172948	9.667853	2.357786
36	1	0	1.376672	9.754957	1.785918
37	1	0	1.888948	9.950330	3.245210
38	8	0	3.480389	8.123692	4.716998
39	1	0	4.409352	8.173849	4.990516
40	1	0	2.963111	8.813042	5.149981
41	8	0	6.160357	7.599716	4.960998
42	8	0	4.449771	10.382968	0.764094
43	8	0	1.284902	9.735983	4.963494
44	8	0	-0.058661	9.463406	0.879917
45	1	0	0.633205	10.234707	5.453820
46	1	0	0.888144	8.871223	4.714199
47	1	0	5.976258	6.650687	5.093622

48	1	0	6.798896	7.858521	5.624780
49	1	0	3.709947	10.522955	1.368189
50	1	0	4.160722	9.585326	0.285469
51	1	0	-0.048220	9.753545	-0.032463
52	1	0	0.123019	8.497920	0.850504
53	6	0	2.440694	2.368745	3.201886
54	1	0	1.650464	2.209419	3.937479
55	1	0	3.384943	2.423990	3.749460
56	6	0	3.386413	2.713884	0.463189
57	1	0	2.470708	2.607623	-0.123623
58	1	0	4.196602	2.884296	-0.245926
59	6	0	3.624813	1.415505	1.223117
60	6	0	2.518955	1.188039	2.243163
61	1	0	2.695663	0.270920	2.806181
62	1	0	1.562470	1.066372	1.726107
63	1	0	4.588926	1.461775	1.738284
64	1	0	3.679916	0.583271	0.520424

E(RwB97XD) = -1827.456389 Hartree; Zero-point correction = 0.515099; Thermal correction to Energy = 0.555326; Thermal correction to Enthalpy = 0.556270; Thermal correction to Gibbs Free Energy = 0.445460; Sum of electronic and zero-point Energies = -1826.941290; Sum of electronic and thermal Energies = -1826.901063; Sum of electronic and thermal Enthalpies = -1826.900119; Sum of electronic and thermal Free Energies = -1827.010929.

Table S8: Cartesian coordinates obtained with DFT calculations for the $[Gd(CDTA)(H_2O)_2]^-\cdot 5H_2O$ system (wB97XD/LCECP/Def2-TZVPP, 0 imaginary frequencies).[a]

Center Number	Atomic Number		Coordinates (Å) X	Y	Z
1	64	0	2.690493	7.198130	2.352353
2	8	0	4.477252	5.932008	3.256998
3	8	0	0.930560	7.298941	3.974502
4	8	0	0.774790	6.898672	1.009152
5	8	0	3.508786	7.845759	0.205622
6	8	0	5.104125	5.024943	5.182374
7	8	0	-0.799291	6.416829	5.059478
8	8	0	0.093874	6.571011	-1.080439
9	8	0	4.766338	7.371232	-1.568973
10	6	0	4.259543	5.262942	4.311909
11	6	0	2.817109	4.830380	4.561413
12	1	0	2.796031	3.884712	5.100919
13	1	0	2.428579	5.581411	5.253205
14	6	0	0.555467	4.951743	3.770078
15	1	0	0.269726	4.183871	4.493625
16	1	0	-0.069873	4.824376	2.885785
17	6	0	0.184725	6.322851	4.337872
18	6	0	4.139494	7.042826	-0.570829
19	6	0	4.141223	5.570303	-0.148945
20	1	0	4.277253	4.957533	-1.042100
21	1	0	5.024689	5.439775	0.480518
22	6	0	1.772347	5.120235	-0.239340
23	1	0	1.161662	4.254003	0.013635
24	1	0	2.052066	4.998755	-1.286106
25	6	0	0.812129	6.302166	-0.125879
26	6	0	2.148577	3.673496	2.449136
27	1	0	1.191635	3.563477	1.936848
28	6	0	3.213294	3.909391	1.368005

29	1	0	4.171426	4.051628	1.865893
30	7	0	2.961015	5.174685	0.628376
31	7	0	1.962441	4.842404	3.364029
32	8	0	6.669383	8.845667	2.581990
33	1	0	5.891525	9.303564	2.228496
34	1	0	6.400966	8.442894	3.415594
35	8	0	1.932876	9.632432	2.241854
36	1	0	1.151449	9.727900	1.654875
37	1	0	1.653901	9.931813	3.124780
38	8	0	3.610404	8.443839	4.331435
39	1	0	4.453154	8.242618	4.778552
40	1	0	3.064142	9.020980	4.878524
41	8	0	6.060501	7.621961	5.183256
42	8	0	4.589304	10.206379	1.173676
43	8	0	1.278983	9.747868	4.914229
44	8	0	-0.274615	9.395922	0.725645
45	1	0	0.670543	10.237116	5.465898
46	1	0	0.898930	8.857647	4.751495
47	1	0	5.909017	6.655656	5.206790
48	1	0	6.474087	7.860906	6.012506
49	1	0	3.780790	10.367139	1.673873
50	1	0	4.327784	9.456821	0.612256
51	1	0	-0.264424	9.659038	-0.194929
52	1	0	-0.068762	8.438233	0.725030
53	6	0	2.404505	2.354730	3.184352
54	1	0	1.624666	2.200002	3.931775
55	1	0	3.356868	2.405711	3.717402
56	6	0	3.336261	2.691778	0.441839
57	1	0	2.423407	2.580318	-0.148037
58	1	0	4.148390	2.862147	-0.264882
59	6	0	3.574434	1.395812	1.205448
60	6	0	2.468852	1.173028	2.226485
61	1	0	2.641854	0.255408	2.789603
62	1	0	1.510298	1.057098	1.712099
63	1	0	4.538727	1.441648	1.720170
64	1	0	3.628199	0.562687	0.503871

E(RwB97XD) = -1827.4561477 Hartree; Zero-point correction = 0.514078; Thermal correction to Energy = 0.554910; Thermal correction to Enthalpy = 0.555854; Thermal correction to Gibbs Free Energy = 0.442243; Sum of electronic and zero-point Energies = -1826.942070; Sum of electronic and thermal Energies = -1826.901238; Sum of electronic and thermal Enthalpies = -1826.900294; Sum of electronic and thermal Free Energies = -1827.013905.

Sample Gaussian input file:

```
%mem=8gb
%chk=freq_Gd_27H2O_wB97XD_2.chk
# rwB97XD/gen pseudo=cards freq=nraman scf=tight opt Integral=superfinegrid
scrf=(read,pcm,solvent=water,iterative) nosymmetry

freq_Gd_27H2O_wB97XD_2

3  1
 Gd             0.17947300    0.11840600    0.08737000
 O              2.16714000   -0.12931300    1.53860100
 H              2.02075500   -0.15467400    2.49917400
 H              2.82084800   -0.83007800    1.33507400
 O              0.16094200    1.88963700    1.82562600
 H              0.86621400    2.25349700    2.38497400
 H             -0.68162100    2.27008700    2.11892800
```

O	1.76801100	-1.31815500	-1.08985700
H	1.61380100	-2.20856600	-1.44556100
H	2.53413400	-0.92504300	-1.55818200
O	0.05692700	-2.15643800	1.11302300
H	0.72977200	-2.85701200	1.07902100
H	-0.80529500	-2.56846800	1.27507300
O	1.89895000	1.72276200	-0.61085200
H	1.74127900	2.42892300	-1.26084700
H	2.53770700	2.06285600	0.05069600
O	0.06342100	0.70453700	-2.46021100
H	0.82077000	0.75827100	-3.06176000
H	-0.69078500	0.38369500	-2.97460400
O	-1.75003600	-0.03975800	1.66492000
H	-1.60052300	-0.19444000	2.61065500
H	-2.57927400	-0.47224300	1.40415000
O	-1.56843000	-1.20681600	-1.01949800
H	-1.56714400	-2.12254500	-1.33731300
H	-2.39316900	-0.78380500	-1.31093400
O	-1.57595300	1.71718800	-0.53884100
H	-1.53539500	2.32714700	-1.29133600
H	-2.42891300	1.82683700	-0.07972300
O	3.97256700	-2.12370900	1.10116400
O	2.01614700	-4.06673200	0.74918800
O	1.62070100	0.02267700	4.25083500
O	-1.12526000	-0.41663500	4.36501800
O	-3.99301500	1.88853800	0.77019200
O	-3.95339700	-0.05439600	-1.86008200
O	3.87462200	-0.08911300	-2.26937000
O	2.29375100	1.40124000	-3.98254200
O	1.25390600	-3.92228900	-1.85078700
O	-1.49087600	-3.79088100	-2.08636300
O	-4.18369300	-1.13993100	0.83980700
O	1.40530400	3.57605600	-2.59994300
O	-1.36980500	3.57556800	-2.63404400
O	3.73115700	2.65906800	1.17480700
O	2.22557900	2.57048300	3.51287700
H	-4.23956500	-1.08439700	-0.12111900
H	-4.02540500	0.85204900	-1.55260900
H	-4.21076300	0.99320500	1.04953200
H	-3.80496100	-2.01028200	1.03634900
H	-3.55162900	-0.00099000	-2.74295500
H	-3.54770500	2.29076400	1.53326900
H	3.29173200	2.62843600	2.04125100
H	4.40104600	1.97527800	1.21477800
H	3.41716800	0.45094700	-2.93760600
H	4.08793100	0.53370000	-1.57192900
H	3.36987100	-2.87088400	0.94357900
H	4.42558500	-1.98572700	0.26856200
H	2.10089200	2.30858800	-3.68652600
H	1.80899600	-4.24248700	-0.18687600
H	2.11486100	1.73295100	3.99749200
H	2.17866400	3.28205800	4.15137200
H	2.33833400	1.41467800	-4.93852700
H	2.03019700	-4.90941700	1.20333700
H	0.43481300	3.64642900	-2.65251500
H	0.29393000	-3.98930700	-2.00022000
H	0.66699900	-0.14044700	4.36241400
H	1.74933200	4.46838600	-2.55170700
H	2.07507000	-0.53976200	4.87869200
H	1.68647700	-4.32004500	-2.60684400

H	-1.71237300	3.25233100	-3.46956100
H	-1.58881200	0.19178700	4.94436400
H	-1.99120700	-4.47565200	-1.63819400
H	-1.81714500	4.40868100	-2.47244300
H	-1.34741900	-1.29466200	4.68247100
H	-1.82037100	-3.77625200	-2.98758400
H	-2.58188600	-3.33267300	2.63842300
H	-2.62543700	-4.16783200	1.36397800
H	-2.44877200	2.88678400	3.60771000
H	-2.24304100	4.02537500	2.61108900
H	-2.32445700	0.48062700	-4.79611700
H	-2.10836800	-0.97798900	-4.39547900
O	-2.27231300	3.06913300	2.68273300
O	-2.20781800	-0.09379000	-4.03677700
O	-2.50343900	-3.27186100	1.68396000

Gd 0
S 3 1.0
7.9250430 -0.1522640
6.2717590 0.4939230
2.5909130 -1.2945530
S 1 1.0
0.6425090 1.0000000
S 1 1.0
0.3128260 1.0000000
S 1 1.0
0.0584800 1.0000000
S 1 1.0
0.0269240 1.0000000
P 3 1.0
5.2050550 0.1141430
3.1110210 -0.4426100
0.7437650 1.1665320
P 1 1.0
0.3127020 1.0000000
P 1 1.0
0.0943750 1.0000000
P 1 1.0
0.0336140 1.0000000
D 3 1.0
2.5342090 -0.0394870
0.8067320 0.3908310
0.3203550 0.7016280
D 1 1.0
0.1242070 1.0000000
D 1 1.0
0.0480910 1.0000000
****
H O 0
Def2tzvpp
****

Gd 0
ECP53MWB 4 53
G-Komponente
1
2 1.000000 0.000000
S-G
2
2 5.026000 139.601619

2 2.513000 -6.879694
P-G
2
2 4.302200 79.873824
2 2.151100 0.938419
D-G
2
2 3.001100 32.709729
2 1.505500 1.241952
F-G
1
2 6.204900 -74.248790

modifysph

O 1.9250 1.0
H 1.5873 1.0

Sample ORCA input file (DFT):

#

DKH2_Gd27H2O_2_TPSSh

#

! uks tpssh tightscf dkh2 RIJCOSX UNO autoaux DKH-def2-TZVPP

%basis

newgto Gd "SARC2-DKH-QZVP" end

newauxcgto Gd "SARC2-DKH-QZVP/JK" end

newauxjkgto Gd "SARC2-DKH-QZVP/JK" end

end

%pal

nprocs 24

end

% maxcore 25000

* xyz 3 8

Gd	0.17945000	0.12079200	0.06310700
O	2.16486100	-0.12002800	1.53094400
H	2.01384200	-0.14093000	2.49073900
H	2.81408800	-0.82658400	1.33442200
O	0.15633600	1.91014800	1.78546500
H	0.85887600	2.26938500	2.35125800
H	-0.68876100	2.27704900	2.08830000
O	1.78421300	-1.33013400	-1.08471200
H	1.62488000	-2.21817200	-1.44398000

H	2.54946100	-0.93873300	-1.55541800
O	0.05890300	-2.14921300	1.10543100
H	0.73037400	-2.85102400	1.07379400
H	-0.80376800	-2.55988400	1.26791300
O	1.91830200	1.71727600	-0.62179100
H	1.76105100	2.42973000	-1.26470800
H	2.55475300	2.05243500	0.04434500
O	0.07410700	0.67466300	-2.41694000
H	0.82813100	0.74671300	-3.02240300
H	-0.68933800	0.38867000	-2.93958500
O	-1.74417100	-0.03444700	1.65774900
H	-1.59088600	-0.19229400	2.60226900
H	-2.57220600	-0.47058600	1.40025700
O	-1.58100700	-1.22015600	-1.01517100
H	-1.57131100	-2.13287800	-1.34142500
H	-2.40621000	-0.80031100	-1.30880100
O	-1.60294000	1.70191600	-0.55442800
H	-1.55738100	2.33482400	-1.28731700
H	-2.44691500	1.81671700	-0.08066800
O	3.96728600	-2.12742500	1.11709900
O	2.01156300	-4.07029600	0.75209100
O	1.61587000	0.04353600	4.24430200
O	-1.12353700	-0.41914300	4.35856000
O	-4.00899900	1.87751100	0.77843900
O	-3.97089900	-0.06494800	-1.85624700
O	3.88661100	-0.09875500	-2.27397900
O	2.26958800	1.37976700	-3.96890300
O	1.25948800	-3.93074400	-1.85220200
O	-1.48335500	-3.79311400	-2.10336300
O	-4.18616400	-1.14404700	0.85053000
O	1.41436700	3.57621400	-2.60413600
O	-1.36135500	3.60009400	-2.60920900
O	3.74718600	2.64911100	1.17114000
O	2.21048700	2.58722000	3.48867700
H	-4.24598600	-1.09422300	-0.11039200
H	-4.03389800	0.83723300	-1.53409000

H	-4.22094200	0.98171600	1.06110800
H	-3.80185000	-2.01143500	1.04973100
H	-3.55861400	0.00062300	-2.73318500
H	-3.55929300	2.28315800	1.53710400
H	3.29686200	2.62747400	2.03232500
H	4.40704600	1.95629600	1.22153500
H	3.42007100	0.43848800	-2.93782500
H	4.09846800	0.52486400	-1.57675800
H	3.36390600	-2.87342400	0.95689600
H	4.42293400	-1.99014200	0.28579400
H	2.08790700	2.29321600	-3.68452700
H	1.80764700	-4.24750000	-0.18434100
H	2.09894600	1.75274700	3.97855900
H	2.16334800	3.30291400	4.12254300
H	2.28924300	1.37559700	-4.92587100
H	2.01917600	-4.91181800	1.20851000
H	0.44425600	3.65722200	-2.64597100
H	0.30008000	-3.99450000	-2.00656200
H	0.66404800	-0.12781700	4.35952800
H	1.76887200	4.46490300	-2.56527800
H	2.07736100	-0.51162300	4.87343600
H	1.69442800	-4.33084100	-2.60564800
H	-1.71854300	3.30262800	-3.44823300
H	-1.59616700	0.18010200	4.94012000
H	-1.98761600	-4.48217900	-1.66626500
H	-1.79211100	4.43729900	-2.42445800
H	-1.33858800	-1.30183700	4.66782300
H	-1.80686300	-3.76725900	-3.00648200
H	-2.57159200	-3.35211600	2.63433400
H	-2.61872200	-4.16367000	1.34447700
H	-2.44229300	2.87625500	3.60049200
H	-2.25572600	4.02349300	2.61004100
H	-2.30546400	0.52610100	-4.76048100
H	-2.08776600	-0.93910600	-4.38564200
O	-2.27839200	3.06660800	2.67484600
O	-2.19062700	-0.06173300	-4.01114500

```
 O              -2.49810900   -3.27347800    1.68079700
*
%cpcm smd true # turn on SMD
SMDsolvent "water" # specify the name of solvent from the list
end
%method
AngularGrid 7
AngularGridX 5
IntAccX 4.5
end
%eprnmr Nuclei= all O {aiso,adip,fgrad}
end
%scf
MaxIter 3000
end
```

Sample ORCA input file (NEVPT2):

```
#
# CASSCF_NO2PP1PA2
#
! RIJCOSX tightscf Normalprint dkh2 autoaux moread DKH-def2-TZVPP
%moinp "DKH2_Gd27H2O_2_TPSSh.qro"
%basis basis "DKH-def2-TZVP"
newgto Gd "SARC2-DKH-QZVP" end
newauxcgto Gd "SARC2-DKH-QZVP/JK" end
newauxjkgto Gd "SARC2-DKH-QZVP/JK" end
end
%pal
  nprocs 30
end
% maxcore 70000
* xyz 3 8
 Gd              0.17945000    0.12079200    0.06310700
 O               2.16486100   -0.12002800    1.53094400
 H               2.01384200   -0.14093000    2.49073900
 H               2.81408800   -0.82658400    1.33442200
```

O	0.15633600	1.91014800	1.78546500
H	0.85887600	2.26938500	2.35125800
H	-0.68876100	2.27704900	2.08830000
O	1.78421300	-1.33013400	-1.08471200
H	1.62488000	-2.21817200	-1.44398000
H	2.54946100	-0.93873300	-1.55541800
O	0.05890300	-2.14921300	1.10543100
H	0.73037400	-2.85102400	1.07379400
H	-0.80376800	-2.55988400	1.26791300
O	1.91830200	1.71727600	-0.62179100
H	1.76105100	2.42973000	-1.26470800
H	2.55475300	2.05243500	0.04434500
O	0.07410700	0.67466300	-2.41694000
H	0.82813100	0.74671300	-3.02240300
H	-0.68933800	0.38867000	-2.93958500
O	-1.74417100	-0.03444700	1.65774900
H	-1.59088600	-0.19229400	2.60226900
H	-2.57220600	-0.47058600	1.40025700
O	-1.58100700	-1.22015600	-1.01517100
H	-1.57131100	-2.13287800	-1.34142500
H	-2.40621000	-0.80031100	-1.30880100
O	-1.60294000	1.70191600	-0.55442800
H	-1.55738100	2.33482400	-1.28731700
H	-2.44691500	1.81671700	-0.08066800
O	3.96728600	-2.12742500	1.11709900
O	2.01156300	-4.07029600	0.75209100
O	1.61587000	0.04353600	4.24430200
O	-1.12353700	-0.41914300	4.35856000
O	-4.00899900	1.87751100	0.77843900
O	-3.97089900	-0.06494800	-1.85624700
O	3.88661100	-0.09875500	-2.27397900
O	2.26958800	1.37976700	-3.96890300
O	1.25948800	-3.93074400	-1.85220200
O	-1.48335500	-3.79311400	-2.10336300
O	-4.18616400	-1.14404700	0.85053000
O	1.41436700	3.57621400	-2.60413600

O	-1.36135500	3.60009400	-2.60920900
O	3.74718600	2.64911100	1.17114000
O	2.21048700	2.58722000	3.48867700
H	-4.24598600	-1.09422300	-0.11039200
H	-4.03389800	0.83723300	-1.53409000
H	-4.22094200	0.98171600	1.06110800
H	-3.80185000	-2.01143500	1.04973100
H	-3.55861400	0.00062300	-2.73318500
H	-3.55929300	2.28315800	1.53710400
H	3.29686200	2.62747400	2.03232500
H	4.40704600	1.95629600	1.22153500
H	3.42007100	0.43848800	-2.93782500
H	4.09846800	0.52486400	-1.57675800
H	3.36390600	-2.87342400	0.95689600
H	4.42293400	-1.99014200	0.28579400
H	2.08790700	2.29321600	-3.68452700
H	1.80764700	-4.24750000	-0.18434100
H	2.09894600	1.75274700	3.97855900
H	2.16334800	3.30291400	4.12254300
H	2.28924300	1.37559700	-4.92587100
H	2.01917600	-4.91181800	1.20851000
H	0.44425600	3.65722200	-2.64597100
H	0.30008000	-3.99450000	-2.00656200
H	0.66404800	-0.12781700	4.35952800
H	1.76887200	4.46490300	-2.56527800
H	2.07736100	-0.51162300	4.87343600
H	1.69442800	-4.33084100	-2.60564800
H	-1.71854300	3.30262800	-3.44823300
H	-1.59616700	0.18010200	4.94012000
H	-1.98761600	-4.48217900	-1.66626500
H	-1.79211100	4.43729900	-2.42445800
H	-1.33858800	-1.30183700	4.66782300
H	-1.80686300	-3.76725900	-3.00648200
H	-2.57159200	-3.35211600	2.63433400
H	-2.61872200	-4.16367000	1.34447700
H	-2.44229300	2.87625500	3.60049200

```
H          -2.25572600   4.02349300   2.61004100
H          -2.30546400   0.52610100  -4.76048100
H          -2.08776600  -0.93910600  -4.38564200
O          -2.27839200   3.06660800   2.67484600
O          -2.19062700  -0.06173300  -4.01114500
O          -2.49810900  -3.27347800   1.68079700
*
%cpcm smd true # turn on SMD
SMDsolvent "water" # specify the name of solvent from the list
end
%method
AngularGrid 7
AngularGridX 5
IntAccX 4.5
end
%rel
picturechange true
FiniteNuc true
end
%casscf
nel 7
norb 7
mult 8,6
nroots 1,48
trafostep ri
PTMethod sc_nevpt2
PTSettings
QDType QD_VanVleck
end
rel
DoSOC true
NInitStates 8
end
end
```