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A Computational Insight into Mechanistic Overview of Water-Exchange Kinetics and Thermodynamic Stabilities of Bis and Tris-Aquated Complexes of Lanthanides†

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Table S1: Binding energy values ($\Delta E_{TOTAL} = E_{COMPLEX} - E_{LIGAND} - E_{Gd(III)}$) and relative binding energy (ΔE_{REL}) values (in kcal/mol) of the chosen complexes were calculated using TPSSh/6-31G(d,p)/SCRECP level of theory.

Methods	**Complex**	**$\Delta E_{total(BSSE\ corrected)}$**	**$\Delta E_{relative}$**
TPSSh/6-31G(d,p)/SCRECP	**Gd(III)-peada**	-197.13	0.0
	Gd(III)-tpaa	-165.73	+31.4
	Gd(III)-cbda	-166.42	0.0
	Gd(III)-dpaa	-165.06	+1.36

Table S2: Binding energy values ($\Delta E_{TOTAL} = E_{COMPLEX} - E_{LIGAND} - E_{Gd(III)}$) and relative binding energy (ΔE_{REL}) values (in kcal/mol) of the chosen complexes using different density functionals and basis sets with LCRECP level of theory.

Methods	**Complex**	**$\Delta E_{total(BSSE\ corrected)}$**	**$\Delta E_{relative}$**
TPSSh/6-31G(d,p)	**Gd(III)-peada**	-157.86	0.00
	Gd(III)-tpaa	-127.51	+30.35
	Gd(III)-cbda	-129.26	0.00
	Gd(III)-dpaa	-127.76	+1.5
TPSSh/6-31+G(d,p)	**Gd(III)-peada**	-113.61	0.0
	Gd(III)-tpaa	-93.67	+19.94
	Gd(III)-cbda	-89.39	0.0
	Gd(III)-dpaa	-87.59	+1.8
TPSSh/def2-TZVP (Single Point Energy)	**Gd(III)-peada**	-126.79	0.0
	Gd(III)-tpaa	-101.32	+25.47
	Gd(III)-cbda	-100.25	0.00
	Gd(III)-dpaa	-98.53	+1.72
B3LYP/6-31G(d,p)	**Gd(III)-peada**	-155.43	0.0
	Gd(III)-tpaa	-114.76	+40.67
	Gd(III)-cbda	-118.68	0.0
	Gd(III)-dpaa	-117.39	+1.29
B3LYP-D3/6-31G(d,p)	**Gd(III)-peada**	-162.74	0.0
	Gd(III)-tpaa	-138.78	+23.96
	Gd(III)-cbda	-140.69	0.0
	Gd(III)-dpaa	-139.29	+1.4
B3LYP-D3/6-31+G(d,p)	**Gd(III)-peada**	-128.03	0.0
	Gd(III)-tpaa	-107.31	+20.72
	Gd(III)-cbda	-111.49	0.0
	Gd(III)-dpaa	-109.89	+1.6
ωB97XD/6-31G(d,p)	**Gd(III)-peada**	-159.45	0.0
	Gd(III)-tpaa	-132.04	+27.41
	Gd(III)-cbda	-134.87	0.0
	Gd(III)-dpaa	-133.28	+1.59

Table S3: Bond length values of the [Gd(tpaa)(H_2O)$_2$] complex using LCRECP and SCRECP with 6-31G(d,p) for H, C, N, O, and TPSSh level of theory.

Complex	**Core-model**	**Gd-O48(W)**	**Gd-O51(W)**	**Gd-N11**	**Gd-N9**	**Gd-N21**	**Gd-N37**	**Gd-O25**	**Gd-O27**	**Gd-O40**
Gd-tpaa	**Large core**	2.774	2.571	2.824	2.616	2.614	2.692	2.351	2.417	2.399
Gd-tpaa	**Small core**	3.72	2.46	2.72	2.50	2.52	2.60	2.27	2.39	2.34

Table S4: Bond length values of the [Gd(peada)(H_2O)$_2$]$^-$ complex using LCRECP and SCRECP with 6-31G(d,p) for H, C, N, O, and TPSSh level of theory.

Complex	**Core-model**	**Gd-O40(w)**	**Gd-O43(w)**	**Gd-N1**	**Gd-N2**	**Gd-N23**	**Gd-O11**	**Gd-O12**	**Gd-O17**	**Gd-O29**
Gd-peada	**Large core**	3.36	2.54	2.65	2.62	2.56	2.34	2.33	2.36	2.42
Gd-peada	**Small core**	3.68	2.47	2.59	2.55	2.49	2.29	2.27	2.31	2.37

Table S5: Bond length values of the [Gd(dpaa)(H_2O)$_3$] complex using LCRECP and SCRECP with 6-31G(d,p) for H, C, N, O, and TPSSh level of theory.

Complex	**Core-model**	**Gd-O36(w)**	**Gd-O39(w)**	**Gd-O43(w)**	**Gd-N1**	**Gd-N9**	**Gd-N15**	**Gd-O7**	**Gd-O12**	**Gd-O14**
Gd-dpaa	**Large core**	2.60	2.59	2.54	2.74	2.61	2.59	2.36	2.41	2.42
Gd-dpaa	**Small core**	2.48	2.52	2.55	2.66	2.53	2.54	2.28	2.38	2.34

Table S6: Bond length (Å) values of the [Gd(cbda)(H_2O)$_3$] complex using LCRECP and SCRECP with 6-31G(d,p) for H, C, N, O, and TPSSh level of theory.

Complex	**Core-model**	**Gd-O36(w)**	**Gd-O39(w)**	**Gd-O47(w)**	**Gd-N1**	**Gd-N9**	**Gd-N15**	**Gd-O7**	**Gd-O12**	**Gd-O14**
Gd-cbda	**Large core**	2.60	2.59	2.54	2.76	2.61	2.59	2.35	2.41	2.43
Gd-cbda	**Small core**	2.48	2.53	2.55	2.68	2.52	2.54	2.28	2.38	2.34

Table S7: Thermodynamic parameters (kcal/mol, scheme 1) were obtained with different density functionals and basis sets for [Gd(cbda)] and [Gd(dpaa)] complexes.

Methods	**$\Delta G^{a}_{(g)}$**	**$\Delta G^{a}_{(sol)}$ [Gd(cbda)]**	**$\Delta G^{b}_{(sol)}$ [Gd(dpaa)]**	**$\Delta G_{(aq)}{}^{c(calcd)}$**	**$\Delta G_{(aq)}{}^{d(exp)}$**
B3LYP/6-31G(d,p)/LCRECP	-6.27	-84.72	-88.48	-1.89	-5.48
B3LYP-D3/6-31G(d,p)/LCRECP	-3.5	-85.45	-87.89	-0.43	-5.48
B3LYP-D3/6-31+G(d,p)/LCRECP	-1.25	-98.312	-101.08	-10.29	-5.48
M06/6-31G(d,p)/LCRECP	-3.76	-88.48	-90.99	-1.25	-5.48
TPSSh/6-31G(d,p)/LCRECP	-3.72	-83.54	-85.45	-1.08	-5.48
TPSSh/6-31+G(d,p)/LCRECP	-4.60	-93.34	-94.13	-7.60	-5.48
ωB97XD/6-31G(d,p)/LCRECP	-4.4	-90.75	-92.51	-11.47	-5.48
B3LYP/6-31G(d,p)/SCRECP	-6.27	-75.30	-75.30	-6.27	-5.48
TPSSh/6-31G(d,p)/SCRECP	-3.83	-69.72	-70.97	-1.88	-5.48

Table S8: Thermodynamic parameters (kcal/mol, scheme S1) were obtained with different density functionals and basis sets for [Gd(peada)]$^{-}$ and [Gd(tpaa)] complexes.

Methods	**$\Delta G^{a}_{(g)}$**	**$\Delta G^{a}_{(sol)}$ [Gd(peada)]$^{-}$**	**$\Delta G^{b}_{(sol)}$ [Gd(tpaa]**	**$\Delta G_{(aq)}{}^{e(calcd)}$**	**$\Delta G_{(aq)}{}^{d(exp)}$**
B3LYP/6-31G(d,p)/LCRECP	-220.17	-91.87	-68.13	-11.70	-9.24
B3LYP-D3/6-31G(d,p)/LCRECP	-227.79	-100.72	-79.86	-15.95	-9.24
B3LYP-D3/6-31+G(d,p)/LCRECP	-222.92	-111.84	-90.21	-8.40	-9.24
M06/6-31G(d,p)/LCRECP	-226.49	-102.96	-79.33	-18.49	-9.24
TPSSh/6-31G(d,p)/LCRECP	-222.29	-99.37	-76.51	-11.52	-9.24
TPSSh/6-31+G(d,p)/LCRECP	-218.44	-107.97	-85.96	-6.26	-9.24
ωB97XD/6-31G(d,p)/LCRECP	-226.59	-104.63	-82.83	-12.84	-9.24
B3LYP/6-31G(d,p)/SCRECP	-220.17	-91.87	-68.13	-11.70	-9.24
TPSSh/6-31G(d,p)/SCRECP	-219.55	-89.19	-65.03	10.09	-9.24

$\Delta G^{a}_{(g)}$ = Change in Gibbs free energy value in gas phase along with BSSE correction using counterpoise method.

$\Delta G^{a}_{(sol)}$ = Calculated in solvent phase with the structure optimized in the gas phase.

$\Delta G^{c}_{(aq)} = \Delta G_{(g)} + \Delta G_{sol}[Gd(cbda)] + \Delta G_{sol}[(dpaa^{3-})] - \Delta G_{sol}[(cbda^{3-})] - \Delta G_{sol}[Gd(dpaa)]$

$\Delta G^{e}_{(aq)} = \Delta G_{(g)} + \Delta G_{sol}[Gd(peada)]^{-} + \Delta G_{sol}[(tpaa^{3-})] - \Delta G_{sol}[(peada^{4-})] - \Delta G_{sol}[Gd(tpaa)]$

$\Delta G_{aq}^{d(exp)} = -RTlnK$, where K is the equilibrium constant. The values of stability constant ($logK_{GdL}$) were mentioned in earlier literature. [1, 2]

Table S9: Ln-O(w) bond lengths (Å) of $[Ln(cbda)(H_2O)_3].6H_2O$ complex using SCRECP/TPSSh/6-31G(d,p) level of theory.

Metal	Ln-O36(w)	Ln-O39(w)	Ln-O47(w)	Ln-N15	Ln-N1	Ln-N9	Ln-O12	Ln-O14	Ln-O7
La	2.572	2.556	2.484	2.756	2.904	2.723	2.515	2.553	2.403
Gd	2.453	2.433	2.364	2.628	2.800	2.643	2.420	2.473	2.295
Lu	2.389	2.361	2.293	2.574	2.795	2.619	2.370	2.411	2.233

Table S10: Ln-O(w) bond lengths (Å) of $[Ln(peada)(H_2O)_2]^{-}.4H_2O$ complex using SCRECP/TPSSh/6-31G(d,p) level of theory.

Metal	Ln-O40(w)	Ln-O43(w)	Ln-N1	Ln-N2	Ln-N23	Ln-O11	Ln-O12	Ln-O17	Ln-O29
La	2.707	2.612	2.796	2.827	2.705	2.445	2.399	2.438	2.535
Gd	2.621	2.506	2.654	2.671	2.535	2.306	2.301	2.338	2.403
Lu	2.580	2.446	2.610	2.624	2.467	2.248	2.243	2.273	2.324

Table S11: Bond length values of the complex $[Gd(cbda)(H_2O)_3].6H_2O$ using LCRECP with different density functionals and basis sets.

Metal	Method	Gd-O36(w)	Gd-O39(w)	Gd-O47(w)	Gd-N15	Gd-N1	Gd-N9	Gd-O12	Gd-O14	Gd-O7
La	**TPSSh/ 6-31G(d,p)**	2.618	2.572	2.555	2.794	2.944	2.779	2.592	2.604	2.473
	TPSSh/ 6-31+G(d,p)	2.661	2.604	2.584	2.804	2.936	2.765	2.582	2.606	2.474
	B3LYP/ 6-31G(d,p)	2.636	2.582	2.573	2.863	3.010	2.835	2.582	2.607	2.476
	B3LYP-D3/ 6-31G(d,p)	2.625	2.571	2.547	2.801	2.964	2.785	2.617	2.607	2.482
	B3LYP-D3/ 6-31+G(d,p)	2.676	2.670	2.572	2.812	2.943	2.755	2.579	2.603	2.482
	ωB97XD/	2.611	2.620	2.538	2.786	2.923	2.746	2.570	2.600	2.481

	6-31G(d,p)									
Gd	**TPSSh/ 6-31G(d,p)**	2.527	2.455	2.421	2.687	2.871	2.703	2.498	2.514	2.351
	TPSSh/ 6-31+G(d,p)	2.562	2.489	2.448	2.678	2.839	2.687	2.495	2.526	2.349
	B3LYP/ 6-31G(d,p)	2.545	2.470	2.431	2.730	2.966	2.745	2.499	2.516	2.353
	B3LYP-D3/ 6-31G(d,p)	2.496	2.485	2.405	2.708	2.89	2.702	2.467	2.518	2.370
	B3LYP-D3/ 6-31+G(d,p)	2.527	2.492	2.430	2.701	2.864	2.692	2.482	2.528	2.362
	ωB97XD/ 6-31G(d,p)	2.507	2.491	2.416	2.686	2.866	2.689	2.467	2.513	2.360
Lu	**TPSSh/ 6-31G(d,p)**	2.433	2.395	2.320	2.624	2.836	2.650	2.407	2.434	2.265
	TPSSh/ 6-31+G(d,p)	2.461	2.433	2.340	2.599	2.796	2.637	2.404	2.444	2.259
	B3LYP/ 6-31G(d,p)	2.464	2.377	2.329	2.690	2.995	2.712	2.421	2.416	2.255
	B3LYP-D3/ 6-31G(d,p)	2.438	2.412	2.316	2.643	2.884	2.666	2.407	2.426	2.268
	B3LYP-D3/ 6-31+G(d,p)	2.465	2.458	2.348	2.612	2.833	2.650	2.408	2.434	2.261
	ωB97XD/ 6-31G(d,p)	2.433	2.410	2.315	2.623	2.850	2.653	2.408	2.425	2.264

Table S12: Bond length values of the complex $[Gd(peada)(H_2O)_2]^{-}.6H_2O$ using LCRECP and with different DFT methods and basis sets.

Metal	**Method**	**Gd-O40(w)**	**Gd-O43(w)**	**Gd-N1**	**Gd-N2**	**Gd-N23**	**Gd-O11**	**Gd-O12**	**Gd-O17**	**Gd-O29**
La	**TPSSh/ 6-31G(d,p)**	2.721	2.658	2.832	2.858	2.740	2.505	2.472	2.509	2.588
	TPSSh/ 6-31+G(d,p)	2.854	2.692	2.836	2.859	2.761	2.530	2.474	2.503	2.625
	B3LYP/ 6-31G(d,p)	2.734	2.691	2.888	2.930	2.768	2.509	2.482	2.512	2.592
	B3LYP-D3/ 6-31G(d,p)	2.743	2.642	2.856	2.866	2.752	2.510	2.479	2.527	2.616
	B3LYP-D3/ 6-31+G(d,p)	2.852	2.693	2.871	2.879	2.773	2.537	2.482	2.513	2.621
	ωB97XD/ 6-31G(d,p)	2.732	2.631	2.846	2.861	2.744	2.508	2.476	2.525	2.606
Gd	**TPSSh/ 6-31G(d,p)**	2.627	2.541	2.723	2.743	2.598	2.395	2.370	2.385	2.450

	TPSSh/ 6-31+G(d,p)	2.709	2.578	2.718	2.732	2.591	2.404	2.368	2.381	2.458
	B3LYP/ 6-31G(d,p)	2.650	2.572	2.77	2.80	2.618	2.405	2.378	2.389	2.452
	B3LYP-D3/ 6-31G(d,p)	2.588	2.531	2.747	2.761	2.604	2.399	2.383	2.395	2.442
	B3LYP-D3/ 6-31+G(d,p)	2.65	2.55	2.750	2.751	2.601	2.413	2.384	2.390	2.454
	ωB97XD/ 6-31G(d,p)	2.60	2.542	2.739	2.753	2.595	2.396	2.377	2.386	2.435
Lu	**TPSSh/6-31G(d,p)**	2.603	2.481	2.656	2.688	2.505	2.267	2.284	2.305	2.356
	TPSSh/ 6-31+G(d,p)	2.716	2.528	2.644	2.671	2.493	2.267	2.277	2.295	2.356
	B3LYP/ 6-31G(d,p)	2.648	2.516	2.717	2.775	2.523	2.263	2.286	2.296	2.351
	B3LYP-D3/ 6-31G(d,p)	2.591	2.492	2.684	2.665	2.499	2.280	2.291	2.312	2.340
	B3LYP-D3/ 6-31+G(d,p)	2.685	2.546	2.672	2.680	2.496	2.273	2.285	2.295	2.349
	ωB97XD/ 6-31G(d,p)	2.584	2.482	2.674	2.677	2.499	2.274	2.290	2.302	2.337

Table S13: Electron density (ρ_{BCP}), electron localization function (ELF), and Laplacian of electron density ($\nabla^2\rho$) at the Ln-O(w) bond critical points calculated for the $[Ln(cbda)(H_2O)_3]\cdot 6H_2O$ system (Ln = La-Lu) at the TPSSh/SCRECP/6-31G(d,p) theoretical level.

Metal	**ρ_{BCP}**			**ELF**			**$\nabla^2\rho$**		
	Ln-O36(w)	**Ln-O39(w)**	**Ln-O47(w)**	**Ln-O36(w)**	**Ln-O39(w)**	**Ln-O47(w)**	**Ln-O36(w)**	**Ln-O39(w)**	**Ln-O47(w)**
La	0.04034	0.04213	0.04822	0.12274	0.12952	0.13703	0.1511	0.1563	0.1888
Gd	0.04338	0.04532	0.05207	0.101	0.10404	0.108	0.1948	0.2048	0.2641
Lu	0.04398	0.04567	0.05103	0.081	0.0901	0.09554	0.2074	0.2239	0.2730

Table S14: Electron density (ρ_{BCP}), electron localization function (ELF), and Laplacian of electron density ($\nabla^2\rho$) at the Ln-O(w) bond critical points calculated for the $[Ln(peada)(H_2O)_3]^-.4H_2O$ system (Ln = La-Lu) at the TPSSh/SCRECP/6-31G(d,p) theoretical level.

Metal	**ρ_{BCP}**		**ELF**		**$\nabla^2\rho$**	
	Ln-O40(w)	**Ln-O43(w)**	**Ln-O40(w)**	**Ln-O43(w)**	**Ln-O40(w)**	**Ln-O43(w)**
La	0.03021	0.03602	0.10764	0.11747	0.1071	0.1363
Gd	0.03595	0.03893	0.09598	0.09986	0.1229	0.1687
Lu	0.02705	0.03623	0.06207	0.07502	0.1153	0.1754

Table S15: Electron density (ρ_{BCP}), electron localization function (ELF), and Laplacian of electron density ($\nabla^2\rho$) at the Ln-O(w) critical points calculated for the $[Gd(cbda)(H_2O)_3].6H_2O$ system at the LCRECP with different density functionals and basis sets.

Metal	**Method**	**ρ_{BCP}**			**ELF**			**$\nabla^2\rho$**		
		Gd-O36 (w)	Gd-O39 (w)	Gd-O47 (w)	Gd-O36 (w)	Gd-O39 (w)	Gd-O47 (w)	Gd-O36 (w)	Gd-O39 (w)	Gd-O47 (w)
La	**TPSSh/ 6-31G(d,p)**	0.03471	0.03892	0.03875	0.09891	0.11222	0.10378	0.1376	0.1536	0.1624
	TPSSh/ 6-31+G(d,p)	0.0311	0.0357	0.0358	0.0904	0.1049	0.0969	0.1224	0.1402	0.1497
	B3LYP/ 6-31G(d,p)	0.0330	0.0375	0.0371	0.0935	0.1065	0.1004	0.1314	0.1502	0.1546
	B3LYP-D3/ 6-31G(d,p)	0.0339	0.0381	0.0394	0.0953	0.1080	0.1044	0.1360	0.1470	0.1663
	B3LYP-D3/ 6-31+G(d,p)	0.0297	0.0307	0.0372	0.0853	0.0921	0.1031	0.1176	0.1183	0.1537
	ωB97XD/ 6-31G(d,p)	0.0345	0.0349	0.0404	0.0934	0.0965	0.1057	0.1419	0.1378	0.1715
Gd	**TPSSh/ 6-31G(d,p)**	0.03755	0.04105	0.04296	0.09674	0.10054	0.1002	0.1450	0.1764	0.1953
	TPSSh/ 6-31+G(d,p)	0.0342	0.0376	0.0393	0.0939	0.1009	0.1012	0.1303	0.1588	0.1799
	B3LYP/ 6-31G(d,p)	0.0355	0.0394	0.0410	0.0952	0.1031	0.0979	0.1379	0.1686	0.1890
	B3LYP-D3/ 6-31G(d,p)	0.0378	0.04181	0.0450	0.09778	0.10985	0.1094	0.1587	0.1784	0.2035
	B3LYP-D3/ 6-31+G(d,p)	0.0340	0.0346	0.0419	0.0913	0.0928	0.1047	0.1443	0.1434	0.1882
	ωB97XD/ 6-31G(d,p)	0.0357	0.0364	0.0433	0.0921	0.0927	0.1025	0.1553	0.1569	0.1993

Lu	**TPSSh/ 6-31G(d,p)**	0.0373	0.04053	0.04708	0.09593	0.10127	0.1091	0.1592	0.1777	0.2209
	TPSSh/ 6-31+G(d,p)	0.0345	0.0367	0.0438	0.0904	0.0953	0.1049	0.1456	0.1573	0.2018
	B3LYP/ 6-31G(d,p)	0.0345	0.0419	0.0447	0.0902	0.1038	0.1008	0.1453	0.1860	0.2150
	B3LYP-D3/ 6-31G(d,p)	0.0365	0.0387	0.0474	0.0938	0.0976	0.1096	0.1566	0.1690	0.2231
	B3LYP-D3/ 6-31+G(d,p)	0.0338	0.0343	0.0435	0.0881	0.0897	0.1042	0.1436	0.1462	0.2012
	ωB97XD/ 6-31G(d,p)	0.0366	0.0385	0.0469	0.0905	0.0937	0.1049	0.1605	0.1717	0.2261

Table S16: Electron density (ρ_{BCP}), electron localization function (ELF), and Laplacian of electron density ($\nabla^2\rho$) at the Ln-O(w) critical points calculated for the $[Gd(peada)(H_2O)_2]^-.4H_2O$ system at the LCRECP and different density functionals and basis sets.

Metal	Method	ρ_{BCP}		ELF		$\nabla^2\rho$	
		Ln-O40(w)	Ln-O43(w)	Ln-O40(w)	Ln-O43(w)	Ln-O40(w)	Ln-O43(w)
La	**TPSSh/6-31G(d,p)**	0.0294	0.0323	0.0923	0.0944	0.1058	0.1243
	TPSSh/6-31+G(d,p)	0.0220	0.0295	0.0728	0.0879	0.0850	0.1130
	B3LYP/ 6-31G(d,p)	0.0283	0.0298	0.0882	0.0875	0.1025	0.1141
	B3LYP-D3/ 6-31G(d,p)	0.0278	0.0322	0.0869	0.0890	0.1002	0.1305
	B3LYP-D3/ 6-31+G(d,p)	0.0216	0.0289	0.0704	0.0842	0.0751	0.*1129*
	ωB97XD/ 6-31G(d,p)	0.0282	0.0329	0.0845	0.0883	0.1043	0.1357
Gd	**TPSSh/ 6-31G(d,p)**	0.0342	0.0364	0.0940	0.0989	0.1106	0.1402
	TPSSh/ 6-31+G(d,p)	0.0310	0.0350	0.0926	0.0976	0.1030	0.1252
	B3LYP/ 6-31G(d,p)	0.0305	0.0349	0.0910	0.0985	0.1036	0.1284
	B3LYP-D3/ 6-31G(d,p)	0.0350	0.0398	0.0959	0.1006	0.1233	0.1449
	B3LYP-D3/ 6-31+G(d,p)	0.0300	0.0335	0.0908	0.0943	0.1018	0.1337
	ωB97XD/6-31G(d,p)	0.0339	0.0411	0.0976	0.0986	0.1185	0.1418
Lu	**TPSSh/ 6-31G(d,p)**	0.0298	0.0334	0.0748	0.086	0.0987	0.1389
	TPSSh/ 6-31+G(d,p)	0.0276	0.0296	0.0587	0.0786	0.0728	0.1203
	B3LYP/ 6-31G(d,p)	0.0236	0.0305	0.0678	0.0806	0.0874	0.1253
	B3LYP-D3/ 6-31G(d,p)	0.0266	0.0320	0.0745	0.0821	0.1021	0.1349
	B3LYP-D3/ 6-31+G(d,p)	0.0212	0.0280	0.0607	0.0741	0.0786	0.1146
	ωB97XD/ 6-31G(d,p)	0.0268	0.0325	0.0724	0.0807	0.1053	0.1400

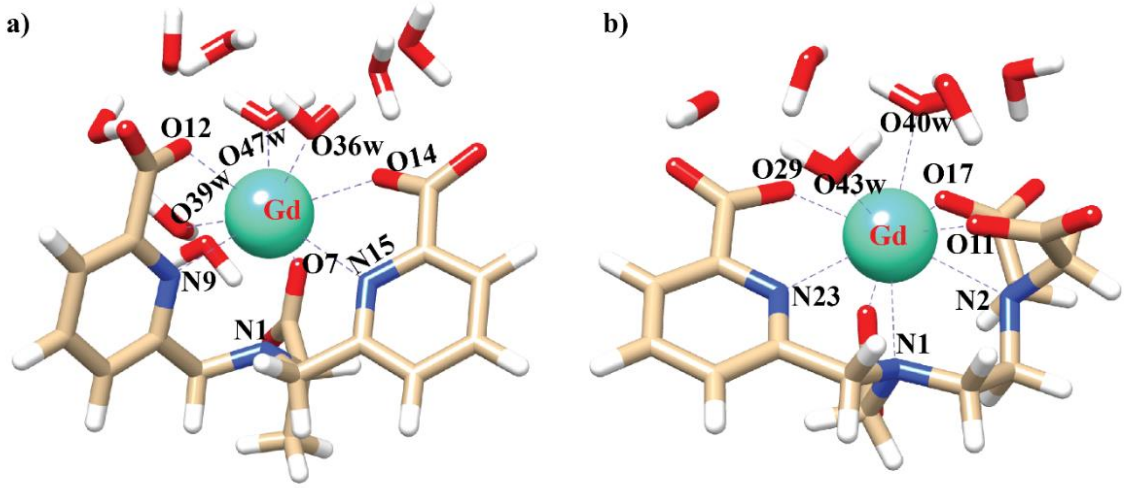


Figure S1: Optimized structures of a) $[Gd(cbda)(H_2O)_3].6H_2O$ and b) $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex using LCRECP/TPSSh/6-31G(d,p) level of theory.

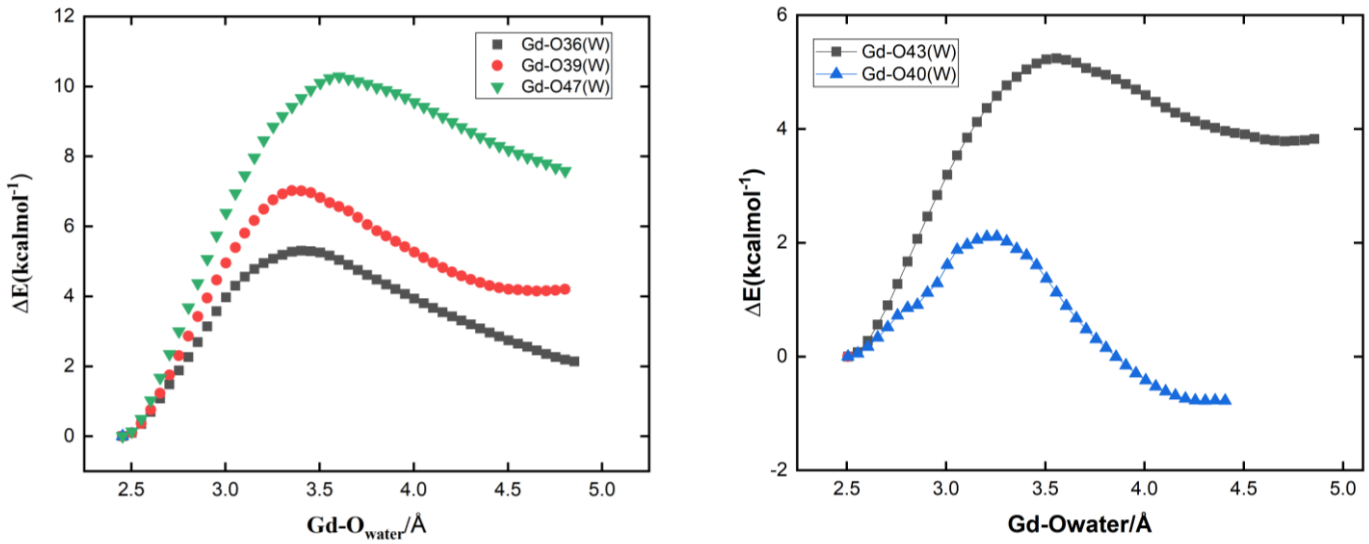


Figure S2: Relaxed potential energy surface scans of the tris-aquated $[Gd(cbda)(H_2O)_3].6H_2O$ and bis-aquated $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex calculated using SCRECP/TPSSh/6-31G(d,p) method.

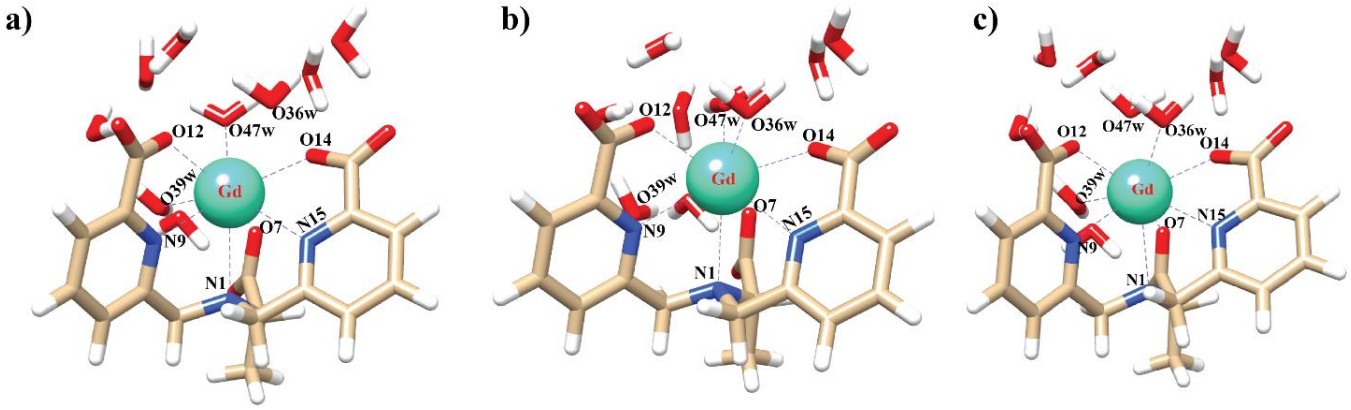


Figure S3: Structure of the transition states (TSs) for the three water molecules of [Gd(cbda)(H_2O)$_3$].6H_2O using LCRECP; (a) TS of Gd-O36(w), (b)TS of Gd-O39(w), and (c) TS of Gd-O47(w).

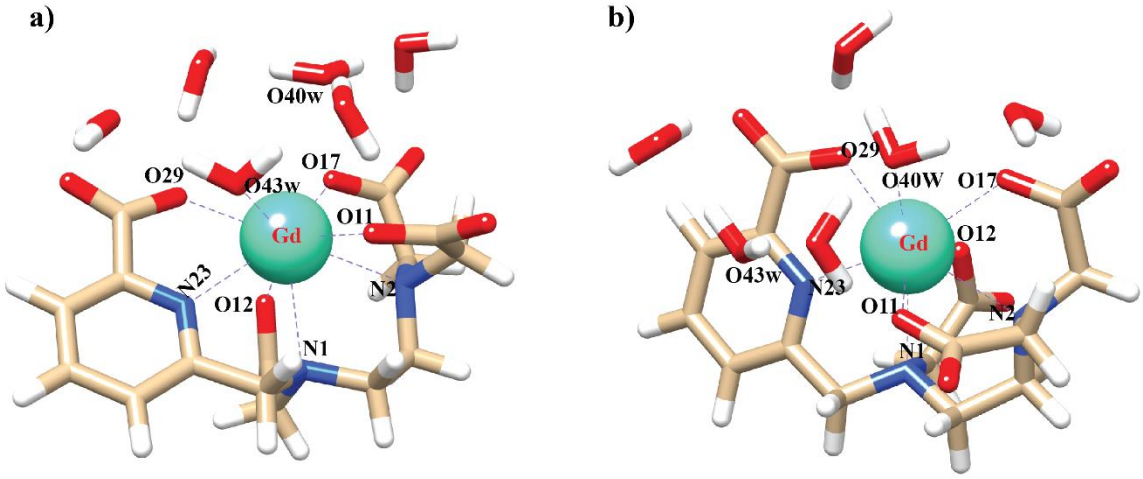


Figure S4: Structure of the transition states (TSs) for the two water molecules of [Gd(peada)(H_2O)$_2$]$^-$.4H_2O complex using LCRECP; a) TS of Gd-O40(w) and b)TS of Gd-O43(w).

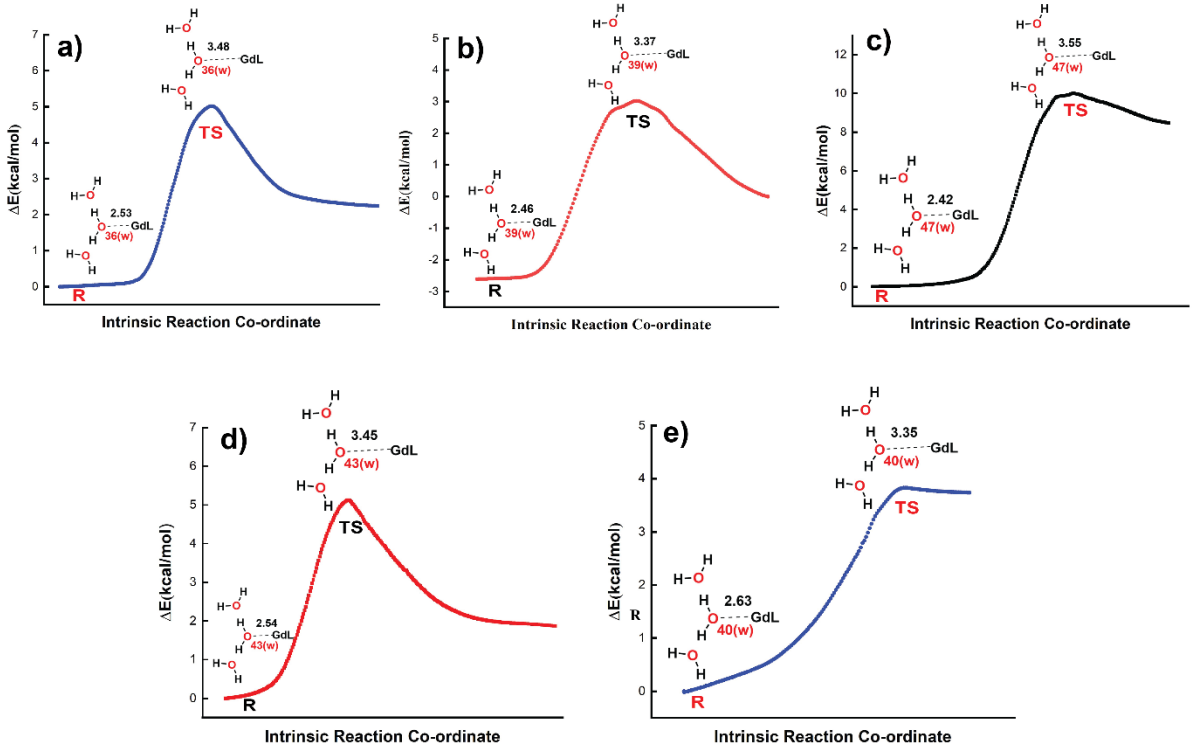
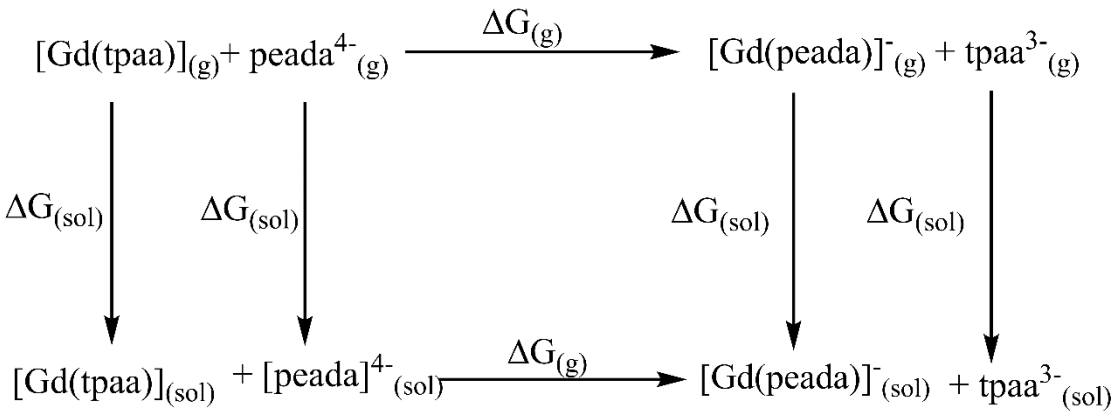


Figure S5: IRC plots for the dissociation of a) Gd-O36(w), b) Gd-O39(w), c) Gd-O47(w), bond of the $[Gd(cbda)(H_2O)_3].6H_2O$ complex (top) and d) Gd-O40(w), e) Gd-O43(w) bond for $[Gd(peada)(H_2O)_2]^-.4H_2O$ (bottom) complexes respectively using LCRECP/TPSSh/6-31G(d,p) level of theory.



Scheme S1. Thermodynamic cycle for explaining the relative stabilities of $[Gd(peada)]^-$ and [Gd(tpaa)] Complexes.

Table S17: Calculated Gd-O(w) bond length, electron density (ρ, au), electron localization function (ELF), and k_{ex}^{298} value of $[Gd(cbda)(H_2O)_3]\cdot 6H_2O$ complex using LCRECP and different density functionals and basis sets.

Method	Ln-Ow bond length	ρ_{BCP}	ELF	k_{ex}^{298} /10^6 S^{-1}
TPSSh/ 6-31G(d,p)	Gd-O36(w)= 2.527	0.0375	0.09674	43.68
	Gd-O39(w)=2.455	0.0410	0.10054	4.2
	Gd-O47(w)= 2.421	0.0429	0.10029	4.6
TPSSh/ 6-31+G(d,p)	Gd-O36(w)= 2.562	0.0342	0.0939	118.9
	Gd-O39(w)=2.489	0.0376	0.1009	6.9
	Gd-O47(w)=2.448	0.0393	0.1012	3.5
B3LYP/ 6-31G(d,p)	Gd-O36(w)= 2.545	0.0355	0.0952	55.5
	Gd-O39(w)=2.470	0.0394	0.1031	2.3
	Gd-O47(w)=2.431	0.0410	0.0979	12.8
B3LYP-D3/ 6-31G(d,p)	Gd-O36(w)= 2.496	0.0378	0.0978	17.8
	Gd-O39(w)=2.485	0.0418	0.10985	0.25
	Gd-O47(w)=2.405	0.0450	0.1094	0.08
B3LYP-D3/ 6-31+G(d,p)	Gd-O36(w)= 2.527	0.0340	0.0913	305.41
	Gd-O39(w)=2.492	0.0346	0.0928	157.14
	Gd-O47(w)=2.430	0.0419	0.1047	3.3
ωB97XD/ 6-31G(d,p)	Gd-O36(w)= 2.507	0.0357	0.0921	173.92
	Gd-O39(w)=2.491	0.0364	0.0927	133.51
	Gd-O47(w)=2.416	0.0433	0.1025	1.6

Table S18: Calculated Gd-O(w) bond length, electron density (ρ, au), electron localization function (ELF), and k_{ex}^{298} value of $[Gd(peada)(H_2O)_2]^{-}\cdot 4H_2O$ complex using LCRECP and different density functionals and basis sets.

Method	Ln-Ow bond length	ρ_{BCP}	ELF	k_{ex}^{298} /10^6 S^{-1}
TPSSh/ 6-31G(d,p)	Gd-O40(w)= 2.627	0.0342	0.0940	118.9
	Gd-O43(w)=2.541	0.0364	0.0989	16.6
TPSSh/ 6-31+G(d,p)	Gd-O40(w)= 2.709	0.0310	0.0926	522.75
	Gd-O43(w)=2.578	0.0350	0.0976	20.48
B3LYP/ 6-31G(d,p)	Gd-O40(w)= 2.650	0.0305	0.0910	944.94
	Gd-O43(w)=2.572	0.0349	0.0985	35.5
B3LYP-D3/ 6-31G(d,p)	Gd-O40(w)= 2.588	0.0350	0.0959	56.6
	Gd-O43(w)=2.531	0.0398	0.1006	4.7
B3LYP-D3/ 6-31+G(d,p)	Gd-O40(w)= 2.650	0.0300	0.0908	1329.08
	Gd-O43(w)=2.550	0.0335	0.0943	140.38
ωB97XD/ 6-31G(d,p)	Gd-O40(w)= 2.60	0.0339	0.0976	75.5
	Gd-O43(w)=2.542	0.0411	0.0986	10.23

Table S19: Activation energy values of $[Gd(cbda)(H_2O)_3].6H_2O$ and $[Gd(peada)(H_2O)_2]^-.4H_2O$ complexes calculated using SCRECP/TPSSh/6-31G(d,p) theoretical level.

	$[Gd(cbda)(H_2O)_3].6H_2O$			**$[Gd(peada)(H_2O)_2]^-.4H_2O$**	
Activation parameters	**Gd-O36(w)**	**Gd-O39(w)**	**Gd-O47(w)**	**Gd-O40(w)**	**Gd-O43(w)**
$\Delta E_a^{\#}$(kcal/mol)	5.33	7.02	10.29	-0.63	5.2
r_{Gd-O}/Å	2.46	2.43	2.36	2.62	2.50
r_{Gd-O}(TS)/Å	3.42	3.34	3.50	2.98	3.54
$\Delta H^{\#}$(kcal/mol)	4.7	6.27	9.78	-0.78	4.26
$\Delta G^{\#}$(kcal/mol)	4.26	5.31	9.16	1.081	3.25
$\Delta S^{\#}$(J/mol/K)	4.19	13.51	8.78	-26.10	13.80

Table S20: Bonding behavior of the $[Gd(cbda)(H_2O)_3].6H_2O$ and $[Gd(peada)(H_2O)_2]^-.4H_2O$ complexes from ETS analysis (in kJ/mol).

Metal	**Ligands**	**ΔE_{int}**	**ΔE_{pauli}**	**ΔE_{oi}**	**ΔV_{elst}**	**[a] %elst**
La	Cbda+H_2O	-5202.50	811.51	-1765.70	-4248.31	70.64
	Peada+ H_2O	-5954.71	732.18	-1733.36	-4953.53	74.07
Lu	Cbda+H_2O	-5618.75	601.31	-1925.46	-4294.60	69.04
	Peada+ H_2O	-6479.69	711.38	-2029.73	-5161.34	71.77

[a] %elst = ΔV_{elst}/ (ΔV_{elst}+ ΔE_{oi})

Table S21: Cartesian coordinates (Å) of [Gd(tpaa)(H_2O)$_2$] complex (without explicit water molecules) optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
C	2.30577300	3.73966400	1.60603400
C	1.67740800	2.50511600	1.40738300
C	1.32093500	2.99074500	-0.83557700
C	1.91816600	4.24379500	-0.71272000
C	2.41742300	4.62444500	0.53339600
H	2.70083100	3.99373400	2.58364300
H	1.98801400	4.87837900	-1.58795700
H	2.89900800	5.58775100	0.66577600
N	1.18892500	2.14342800	0.20639100
C	1.47786300	1.52235200	2.53715800
N	1.53175000	0.12321700	2.04586900
C	0.91706300	-0.79978400	3.03345100
C	-1.27067400	-0.66158100	4.35575100
C	-2.61602400	-0.28902100	4.39385200
C	-3.20080800	0.27485100	3.25833500
C	-2.42138500	0.41263300	2.11079300
C	-0.55804000	-0.49261000	3.16459200
H	-0.77547600	-1.06076200	5.23424300
H	-3.18993600	-0.41174800	5.30657400
H	-4.22855000	0.61727900	3.24269400
N	-1.13835000	0.00989400	2.06110300
C	-2.94662200	1.06363800	0.84664700
C	0.80286200	2.49539400	-2.17085000
O	0.83657900	3.24437900	-3.15218400
O	0.36324700	1.27154600	-2.15447000
O	-4.11913900	1.45293400	0.80459600
O	-2.06572700	1.15855400	-0.10491300
C	2.94667400	-0.23968000	1.80881000
C	3.08236000	-1.49048800	0.97722600
C	4.15015000	-2.37781700	1.14978200
C	4.25973100	-3.47711600	0.29760200
C	3.29641000	-3.66165700	-0.69438800
C	2.25372500	-2.74075800	-0.79103600
H	4.87587200	-2.20489900	1.93713000
H	5.07926000	-4.17923100	0.41143900
H	3.32273400	-4.49609300	-1.38471900
N	2.14860800	-1.67469400	0.02713200
C	1.15997800	-2.89767200	-1.82723200
O	1.21032900	-3.84815300	-2.61675600
O	0.23399300	-1.98789100	-1.78239400
H	1.06047000	-1.82245100	2.66566100
H	1.40759100	-0.73139300	4.01480400

H	2.21808200	1.69703500	3.33002200
H	0.48983700	1.69476100	2.97375900
H	3.40679800	0.59000000	1.25927800
H	3.49575500	-0.34603100	2.75494600
Gd	-0.02341800	-0.11908800	-0.29920500
O	-1.87007100	-0.11680100	-2.36852600
H	-2.33022200	0.53383000	-1.79423800
H	-1.20430500	0.43057600	-2.83143200
O	-1.78438800	-1.98541300	-0.14260600
H	-2.69186300	-1.73545300	-0.37310100
H	-1.39372300	-2.34911000	-0.96901000

E = -1668.864651Hartree

Zero-point correction = 0.389638 Hartree/particle

Sum of electronic and thermal Energies = -1668.443462 Hartree

Sum of electronic and thermal Enthalpies = -1668.442518 Hartree

Sum of electronic and thermal Free Energies = -1668.537182 Hartree

Table S22. Cartesian coordinates (Å) of [Gd(dpaa)(H_2O)$_3$] complex (without explicit water molecules) optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	3.01838600	-0.12670100	1.18555900
C	3.86035700	0.34878300	0.05956100
H	4.93033300	0.20495200	0.26421600
H	3.69122100	1.42676900	-0.05231800
C	3.30501700	-1.54792600	1.50537300
C	2.10191500	-2.27449100	2.13096600
O	0.93009200	-1.82479600	1.77424800
O	2.30475800	-3.24312400	2.86629300
N	1.38128700	2.06561700	1.69077100
C	2.57313600	2.04595300	2.31333800
C	-0.71036400	3.13142700	1.03051000
O	-1.00181500	1.98149500	0.49772800
O	-1.43174200	4.13555600	1.03540400
O	-0.31501200	-1.60174300	-1.24727900
N	2.18663700	-0.75849000	-1.29415600
C	3.47126400	-0.36706800	-1.21581400
C	3.26120900	0.70220700	2.38763200
H	2.84289400	0.16106100	3.24475300
H	4.33602700	0.82660200	2.57877700
C	3.09785600	3.18461700	2.93437600
C	2.34895400	4.36225300	2.92934700

C	1.09686900	4.36815500	2.31335800
C	0.64965200	3.19773500	1.70131000
C	4.38353800	-0.63952700	-2.24014500
C	3.94446100	-1.34109900	-3.36453400
C	2.62021700	-1.77963900	-3.42146000
C	1.77157900	-1.47115400	-2.35939200
C	0.33107400	-1.95053900	-2.31746600
O	-0.11077300	-2.61692200	-3.26118100
H	5.41546500	-0.31843200	-2.14865600
H	4.63401400	-1.56256100	-4.17263500
H	2.23389000	-2.35684500	-4.25288400
H	4.06954800	3.14206400	3.41440300
H	2.73553900	5.25856200	3.40347200
H	0.46252700	5.24603500	2.29120500
O	-0.18047400	1.21967200	-1.82633700
H	-0.73080400	0.70806300	-2.43811200
H	-0.78475400	1.82574200	-1.34612000
O	-0.63237100	0.00907500	2.78022400
H	-0.27176200	-0.88860900	2.93905900
H	-1.59223200	-0.10861100	2.70320100
H	3.53522300	-2.07375900	0.57376200
O	-2.04164900	-0.70083400	0.40761800
H	-1.95232900	-1.24587600	-0.40424500
H	-2.62438800	0.04448100	0.19090500
Gd	0.39504900	0.01713800	0.40752200
H	4.17799400	-1.64566100	2.16153800

E = -1498.091303 Hartree

Zero-point correction = 0.34816 Hartree/particle

Sum of electronic and thermal Energies = -1497.714261 Hartree

Sum of electronic and thermal Enthalpies = -1497.713317 Hartree

Sum of electronic and thermal Free Energies = -1497.801429 Hartree

Table S23: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	2.95004600	-0.23185300	1.26376300
C	3.82156100	0.34290200	0.21606900
H	4.88923100	0.19938900	0.43598100
H	3.64547800	1.42478700	0.19436000
C	3.23765500	-1.68552900	1.49111600
C	1.94772800	-2.32900200	2.04299600
O	0.89373000	-2.12298100	1.33987600

O	1.97999700	-3.00196200	3.09806300
N	1.39004100	2.02307300	1.61714500
C	2.52012500	1.93637400	2.33696700
C	-0.53642200	3.18548100	0.77743200
O	-1.08632500	2.02182900	0.72617500
O	-1.02244500	4.24315200	0.32045900
O	-0.16823500	-1.76155500	-1.44184300
N	2.22019800	-0.62899300	-1.32085300
C	3.49356500	-0.24140800	-1.13693000
C	3.08412000	0.54739100	2.51073300
H	2.50260800	0.03284400	3.28445000
H	4.12484500	0.61069700	2.85586700
C	3.10722000	3.06127300	2.92892100
C	2.50890000	4.30987400	2.75444800
C	1.33030200	4.39766300	2.01191600
C	0.79667000	3.22335900	1.48130800
C	4.46395000	-0.39169200	-2.13535600
C	4.09528100	-0.94838200	-3.35970700
C	2.77888200	-1.37768500	-3.53883500
C	1.88110100	-1.21592100	-2.48462600
C	0.46473600	-1.72796500	-2.55738700
O	0.00548500	-2.07174600	-3.67330700
H	5.48669200	-0.08323000	-1.94626500
H	4.82816700	-1.06710900	-4.15110400
H	2.43993500	-1.84364400	-4.45618600
H	4.01833700	2.95392600	3.50780300
H	2.95299500	5.19699800	3.19419800
H	0.81522400	5.33716500	1.85043000
O	-0.76294300	0.87289600	-1.73607800
H	-1.30369400	0.27298300	-2.30334500
H	-1.30658800	1.70548600	-1.66870500
O	-0.24307200	-0.08068500	2.79967300
H	-0.40346700	-0.97045500	3.22237100
H	-0.97891100	0.52530900	3.08755800
H	3.36741500	-2.11374400	0.49160600
C	4.47971400	-1.99615200	2.32866700
H	4.66684800	-3.07245400	2.29940900
H	5.36651200	-1.48956900	1.93390500
H	4.34443700	-1.71415900	3.37547200
O	-2.02767200	-0.96087900	0.58506900
H	-2.42162500	-1.56443100	-0.11139600
H	-2.73197400	-0.75772200	1.23916300
O	-0.53318700	-2.50198700	3.98257100
H	-0.41302100	-2.37531100	4.93550800
H	0.34585500	-2.84612000	3.66344400
O	-2.31426700	1.59998300	3.19775700
H	-2.09646000	1.89327100	2.28686000
H	-3.06403700	0.98154900	3.06447700
O	-4.05846900	-0.41508800	2.39408700
H	-4.24526600	-1.14641300	3.00231600

H	-4.90579100	-0.20906900	1.97075400
O	-2.75366800	-2.59896700	-1.36375900
H	-1.77369000	-2.59749000	-1.48887100
H	-3.01472500	-1.99524000	-2.09187400
O	-2.32375800	-0.79180200	-3.37787800
H	-2.68419800	-0.39351900	-4.18320300
H	-1.56312100	-1.36750000	-3.66329400
O	-2.32160800	3.11096300	-1.78708300
H	-2.00550900	3.64083600	-2.53394200
H	-1.99946600	3.59942900	-0.98559200
Gd	0.21988800	-0.08132600	0.38827400

E = -1996.134446 Hartree

Zero-point correction = 0.526378 Hartree/particle

Sum of electronic and thermal Energies = -1995.563060 Hartree

Sum of electronic and thermal Enthalpies = -1995.562116 Hartree

Sum of electronic and thermal Free Energies = -1995.684032 Hartree

Table S24: Cartesian coordinates (Å) of $[Gd(cbda)(H_2O)_3].6H_2O$ complex, optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	2.82766200	-0.21901000	1.27228500
C	3.77278700	0.28271900	0.24857400
H	4.82055000	0.08620200	0.51691700
H	3.65577300	1.37152300	0.19662500
C	3.02681000	-1.68182500	1.54480000
C	1.67951400	-2.23898300	2.04657400
O	0.66501000	-1.95963100	1.31796900
O	1.62893000	-2.91869100	3.10074400
N	1.35429100	2.09443700	1.52792500
C	2.46318800	1.99205900	2.27716400
C	-0.57580900	3.25435200	0.71186700
O	-1.07461400	2.07809100	0.58518400
O	-1.11060700	4.32198800	0.33443900
O	-0.24939100	-1.63976800	-1.44645600
N	2.17483500	-0.63899600	-1.30924400
C	3.46157500	-0.31547500	-1.09985800
C	2.96879900	0.58836300	2.50107900
H	2.34274300	0.12834500	3.27453900
H	4.00307700	0.61359500	2.86922400
C	3.05702400	3.11041100	2.87477900
C	2.47669900	4.36620200	2.68860100
C	1.30033300	4.46412700	1.94355700

C	0.76402300	3.29622800	1.40161900
C	4.45021200	-0.54579800	-2.06426600
C	4.08625300	-1.12007300	-3.28206300
C	2.75477700	-1.48796700	-3.48503200
C	1.83875900	-1.24700300	-2.46260200
C	0.40395000	-1.69673000	-2.54747900
O	-0.04651600	-2.07877000	-3.65532800
H	5.48237200	-0.28664000	-1.85409300
H	4.83319800	-1.30141000	-4.04802800
H	2.41686900	-1.96810900	-4.39546800
H	3.95580400	2.99258500	3.47063100
H	2.92709100	5.24911100	3.13058400
H	0.78760000	5.40619000	1.78932400
O	-0.63455600	0.97877100	-1.80487100
H	-1.19224200	0.40854900	-2.38474800
H	-1.13156200	1.83905800	-1.76647600
O	-0.25764700	0.17160900	2.68439500
H	-0.40616000	-0.67074200	3.17649100
H	-1.02326400	0.76319900	2.90794400
H	3.17683800	-2.14064900	0.56182200
C	4.21036300	-2.03863300	2.44503600
H	4.32955800	-3.12480800	2.45910800
H	5.14254600	-1.60215600	2.07218600
H	4.05076300	-1.71151900	3.47515100
O	-2.03525900	-0.64309900	0.52245500
H	-2.45983900	-1.19185300	-0.19655300
H	-2.38531900	-0.98965100	1.38103300
O	-0.74904300	-2.22267300	4.01947600
H	-0.59718700	-2.12485400	4.97054500
H	0.07686000	-2.66255700	3.64766100
O	-2.62646800	1.45371700	2.86427100
H	-2.46014400	1.63644800	1.91635300
H	-3.04646600	0.56971300	2.88487700
O	-3.04788100	-1.36365000	2.91755800
H	-2.30462700	-1.82471900	3.38214300
H	-3.78721400	-1.98676700	2.88048500
O	-2.88799500	-2.26508500	-1.41603500
H	-1.90750000	-2.35223700	-1.50204800
H	-3.07150700	-1.67308600	-2.17620300
O	-2.26032200	-0.58434700	-3.48553400
H	-2.55615600	-0.17095600	-4.30920300
H	-1.54699200	-1.23188100	-3.73387600
O	-2.12970700	3.27805700	-1.96588900
H	-1.67931700	3.83975500	-2.61402500
H	-1.93870000	3.71683300	-1.09724500
Gd	0.21443700	0.04870500	0.30063200

E= -2725.566017 Hartree

Zero-point correction = 0.528291 Hartree/particle

Sum of electronic and thermal Energies = -2724.993756 Hartree

Sum of electronic and thermal Enthalpies = -2724.992812 Hartree

Sum of electronic and thermal Free Energies = -2725.113212 Hartree

Table S25: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.32368500	-2.40870000	0.61229000
N	2.42950900	-1.38619900	0.04469400
C	0.89181700	-2.94773700	1.26545100
C	2.10662200	-2.80319600	0.34880200
C	-0.65372600	-3.20920600	-0.59755500
C	3.27612500	-0.80163600	1.10946000
C	-0.11804900	-2.60643900	-1.90560400
C	2.48808200	-0.23589800	2.29616200
O	0.11644900	-3.37234000	-2.85504000
O	3.06940100	-0.06261100	3.37426800
O	1.25528600	0.09809500	2.04903400
O	-0.00091800	-1.32236100	-1.91826000
C	3.11259200	-1.24938200	-1.26488100
C	3.06074000	0.22482800	-1.69136500
C	-1.47653800	-2.40160400	1.54076500
O	4.11050000	0.80453800	-2.05896900
O	1.91160100	0.78784200	-1.60866600
C	-2.63193100	-1.66619800	0.89104400
C	-3.97275800	-2.01636900	1.08423600
C	-4.96438200	-1.26677400	0.44720700
C	-4.59421200	-0.18454000	-0.35298400
C	-3.23467800	0.09722500	-0.49708500
N	-2.28289700	-0.63652000	0.10213200
H	-6.01076000	-1.52399600	0.57591200
H	-4.22907400	-2.86183100	1.71376600
H	-5.32242500	0.44057500	-0.85572000
C	-2.74693400	1.30898400	-1.26636800
O	-3.58483400	2.15939500	-1.63081500
O	-1.46877900	1.40212400	-1.42469100
H	1.04073800	-2.40471500	2.20133100
H	0.76283000	-4.01422100	1.50941100
H	2.96705000	-3.30698700	0.81289100
H	1.91217400	-3.31686600	-0.59669300
H	4.15176200	-1.60141000	-1.23008800
H	2.55621600	-1.83633600	-2.00104300
H	4.02524700	-1.51935400	1.46977600
H	3.82491100	0.04721500	0.68431700
H	-1.78352400	-3.41684900	1.83011800

H	-1.17366700	-1.87297400	2.45283600
O	1.05677400	2.63030200	0.22429900
H	0.47399700	3.22686200	-0.32401100
H	1.96660600	2.74436900	-0.17158100
O	-1.21661900	1.42419100	1.62915300
H	-0.61491600	1.95673200	2.21408900
H	-1.97440200	2.01660800	1.39978600
H	-1.74238500	-3.24741500	-0.70616900
H	-0.30755800	-4.24469600	-0.49046300
O	3.50829800	3.17792900	-0.83712000
H	4.18623100	3.19044900	-0.14569900
H	3.74654500	2.39546600	-1.40221400
O	0.78160000	2.66813000	2.94140900
H	1.10142800	1.73978700	2.98798200
H	1.01433800	2.88788000	2.00706500
O	-3.32966400	3.12904400	1.05767000
H	-3.59040700	2.99856900	0.12266000
H	-4.09818100	2.83235900	1.56743400
O	-0.60380300	3.95556300	-1.42050000
H	-1.02538800	3.07909500	-1.61759400
H	-0.12802500	4.19484000	-2.22966200
Gd	0.17818700	0.17420500	-0.08925900

E = -1841.788663 Hartree

Zero-point correction = 0.458929 Hartree/particle

Sum of electronic and thermal Energies = -1841.291017 Hartree

Sum of electronic and thermal Enthalpies = -1841.290073 Hartree

Sum of electronic and thermal Free Energies = -1841.399218 Hartree

Table S26: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.32101800	-2.45499800	0.57998800
N	2.40347800	-1.36122000	0.05589000
C	0.89663200	-2.98374300	1.23923900
C	2.12018500	-2.78968000	0.34587300
C	-0.66876800	-3.27412300	-0.61213000
C	3.17992600	-0.72135000	1.14798400
C	-0.23915400	-2.64352900	-1.94598300
C	2.29097000	-0.06673100	2.21447300
O	-0.20123300	-3.37424000	-2.94970600
O	2.83060000	0.51014800	3.17903200
O	1.02386100	-0.11424100	2.00071700
O	0.01157600	-1.38017000	-1.91504900
C	3.12321400	-1.20729300	-1.23151200

C	3.00441600	0.25297100	-1.68276400
C	-1.46068900	-2.40631200	1.52365600
O	4.02143100	0.86616500	-2.08998100
O	1.83636800	0.76531600	-1.58292700
C	-2.62102600	-1.69461000	0.86027600
C	-3.96444700	-2.02282600	1.07158600
C	-4.95122300	-1.26432900	0.43634900
C	-4.57453000	-0.18985800	-0.37186700
C	-3.21271800	0.06700500	-0.53617200
N	-2.26794000	-0.68459300	0.04953700
H	-5.99994500	-1.50385700	0.57974500
H	-4.22755900	-2.85411400	1.71686100
H	-5.29959600	0.44926400	-0.86142900
C	-2.69755500	1.28032000	-1.28124100
O	-3.51277100	2.15813700	-1.63457000
O	-1.41712200	1.34876300	-1.41697600
H	1.02186300	-2.45482900	2.18498400
H	0.78612500	-4.05809000	1.45547800
H	2.98960400	-3.27237000	0.81623200
H	1.95473600	-3.29558100	-0.60959100
H	4.17575500	-1.51077600	-1.16412000
H	2.61633800	-1.82728200	-1.97634200
H	3.87217700	-1.43039300	1.62335700
H	3.79575700	0.07692600	0.71992000
H	-1.76325300	-3.40535600	1.86841500
H	-1.14200100	-1.82582100	2.39793100
O	1.03913800	2.48662600	0.31617400
H	0.42401700	3.10524300	-0.16296300
H	1.91389000	2.66139200	-0.12958300
O	-1.17487000	1.30467600	1.60043800
H	-0.52943500	1.70477900	2.23633000
H	-1.81941900	2.01592600	1.37402300
H	-1.75659000	-3.38749700	-0.66154500
H	-0.25499900	-4.28669400	-0.52937800
O	3.35900200	3.24433000	-0.93895200
H	4.07232500	3.29845600	-0.28603800
H	3.60318000	2.45794900	-1.49729100
O	0.81022600	2.62556800	3.04902300
H	1.40118600	1.87882700	3.29093900
H	1.03312100	2.75882800	2.09650600
O	-3.08878100	3.26816300	0.98674700
H	-3.34028700	3.11386200	0.05282400
H	-3.86963200	2.98922900	1.48798200
O	-0.56798400	3.91378500	-1.34289500
H	-0.98084700	3.04094300	-1.57067200
H	0.04416400	4.09003400	-2.07320400
Gd	0.14866100	0.06071100	-0.12627700

E = -2571.215711 Hartree

Zero-point correction = 0.460043 Hartree/particle

Sum of electronic and thermal Energies = -2570.717284 Hartree

Sum of electronic and thermal Enthalpies = -2570.716340 Hartree

Sum of electronic and thermal Free Energies = -2570.826393 Hartree

Table S27: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, corresponding to Gd-O36(w) bond optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	2.98410800	-0.28789200	1.34107400
C	3.88011500	0.26622200	0.30036700
H	4.93993900	0.08953700	0.53016400
H	3.73729700	1.35289700	0.28092900
C	3.27826800	-1.73855900	1.59111200
C	1.98236100	-2.39429800	2.11098500
O	0.94332800	-2.19522100	1.37816000
O	1.99148000	-3.06748300	3.16348300
N	1.41194000	1.96741200	1.61803600
C	2.52944100	1.90166100	2.36051300
C	-0.48830800	3.10112300	0.67330800
O	-1.01613500	1.92700800	0.59558000
O	-0.97873400	4.15777600	0.22408700
O	-0.18631500	-1.59584300	-1.43962100
N	2.26010300	-0.63145000	-1.26306300
C	3.54470800	-0.29327400	-1.06159700
C	3.09331400	0.51743000	2.57793800
H	2.49677300	0.01787500	3.34965300
H	4.12731900	0.58991700	2.93917400
C	3.10409900	3.04629200	2.92503800
C	2.50690300	4.28735000	2.69731800
C	1.34483300	4.35131000	1.92661200
C	0.82261700	3.16087200	1.42156300
C	4.51257400	-0.44715700	-2.06190400
C	4.12698900	-0.94391600	-3.30675900
C	2.79313200	-1.30339000	-3.51078600
C	1.89788000	-1.14556700	-2.45477800
C	0.45526200	-1.57480200	-2.55339900
O	-0.00962300	-1.88351100	-3.67331200
H	5.54545600	-0.18384200	-1.86070500
H	4.85869900	-1.06465600	-4.09884700
H	2.43880900	-1.71111400	-4.44979600
H	4.00528000	2.96117900	3.52261700
H	2.94191100	5.18889500	3.11618800
H	0.83549200	5.28532800	1.72167900
O	-0.94198100	1.27003800	-2.45282300

H	-1.53154400	0.59455800	-2.84497400
H	-1.55232000	1.99033200	-2.17021900
O	-0.15698300	-0.12713300	2.86101200
H	-0.34917300	-1.00761500	3.29420200
H	-0.88702100	0.50323600	3.11625600
H	3.43977200	-2.17181600	0.59782400
C	4.49921700	-2.02866000	2.46519600
H	4.69399400	-3.10380600	2.45479000
H	5.39268100	-1.52096600	2.08778500
H	4.33313700	-1.73373900	3.50391700
O	-1.96886300	-0.96010500	0.62359300
H	-2.38386200	-1.52916800	-0.09058200
H	-2.65376300	-0.79377700	1.30818600
O	-0.52157400	-2.52813200	4.03061900
H	-0.41324900	-2.41830600	4.98712200
H	0.34980500	-2.89644200	3.72054900
O	-2.20090600	1.58870700	3.13614900
H	-2.01313000	1.82684700	2.20356200
H	-2.95760100	0.96765300	3.06680100
O	-3.94472700	-0.47596200	2.51021800
H	-4.08020900	-1.19054700	3.15115400
H	-4.81551300	-0.31289100	2.11680600
O	-2.74099400	-2.53780900	-1.35459300
H	-1.76462100	-2.52387500	-1.48698700
H	-3.01634500	-1.96795500	-2.10815500
O	-2.50870100	-0.89112200	-3.53502300
H	-2.95468300	-0.81317900	-4.39056100
H	-1.65283400	-1.36854300	-3.71133900
O	-2.67168500	3.36762500	-1.76202700
H	-2.48915400	4.02172400	-2.45258500
H	-2.15266900	3.69154200	-0.98101000
Gd	0.30604700	-0.14868400	0.46612100

E = -1996.126602 Hartree

Zero-point correction =0.525290 Hartree/particle

Sum of electronic and thermal Energies = -1995.556321 Hartree

Sum of electronic and thermal Enthalpies = -1995.555377 Hartree

Sum of electronic and thermal Free Energies = -1995.677654 Hartree

Table S28: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, corresponding to Gd-O39(w) bond optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	2.79121300	-0.20155100	1.23500700
C	3.76956700	0.26938500	0.22780600
H	4.80642700	0.05978700	0.52597500

H	3.67232600	1.36005700	0.16490900
C	2.93914200	-1.66432500	1.52832800
C	1.58666200	-2.17349100	2.07339900
O	0.55287900	-1.86214600	1.37776200
O	1.55269400	-2.86517600	3.11602600
N	1.28009600	2.10837900	1.53123100
C	2.40645900	2.00652400	2.25641300
C	-0.61732400	3.29683600	0.65973300
O	-1.14280700	2.13050500	0.51239400
O	-1.10407700	4.36976300	0.24189700
O	-0.21913000	-1.62919600	-1.57877500
N	2.20827700	-0.64272100	-1.37779500
C	3.49116500	-0.33429800	-1.12599400
C	2.93470000	0.60978700	2.46291200
H	2.31581000	0.15000900	3.24028800
H	3.97480400	0.64852900	2.81289500
C	3.00277400	3.12533200	2.85080900
C	2.41394600	4.37923900	2.68411300
C	1.23523500	4.48037800	1.94326700
C	0.69686300	3.31501300	1.39941600
C	4.50589400	-0.58261300	-2.05832400
C	4.17185000	-1.15217500	-3.28681400
C	2.84188500	-1.49874900	-3.53506100
C	1.89790400	-1.24474600	-2.54227800
C	0.45735700	-1.66828800	-2.67074300
O	0.02177300	-2.01374700	-3.79320500
H	5.53478800	-0.33894500	-1.81615800
H	4.94042000	-1.34541400	-4.02795500
H	2.52796400	-1.97159800	-4.45781800
H	3.91246200	3.00787800	3.42998800
H	2.86492100	5.26033400	3.12900400
H	0.72645600	5.42421400	1.78765900
O	-0.74450000	1.00615300	-1.95385700
H	-1.28209600	0.42445600	-2.54533700
H	-1.24409500	1.86960300	-1.91679600
O	0.05860400	0.28275500	3.54446100
H	-0.23585600	-0.60637500	3.83157600
H	-0.78074500	0.79239800	3.44966400
H	3.05275500	-2.14719800	0.55132500
C	4.12793800	-2.04934100	2.41115900
H	4.20402700	-3.13862400	2.44845600
H	5.06746500	-1.65900500	2.00731800
H	4.00533400	-1.69131900	3.43597500
O	-2.10373300	-0.65979900	0.44910200
H	-2.48741300	-1.26308200	-0.25321000
H	-2.43022700	-0.98768700	1.32785500
O	-0.83350300	-2.36346800	4.14908700
H	-0.80272100	-2.61192600	5.08328900
H	0.00876000	-2.70775000	3.72353700
O	-2.40260100	1.44235800	3.00922100

H	-2.15885000	1.62431100	2.07865700
H	-2.79846900	0.54513100	2.99761100
O	-2.94306600	-1.31669500	2.90478600
H	-2.22354800	-1.80105200	3.39359000
H	-3.75062600	-1.84249000	2.99088300
O	-2.84324300	-2.30817800	-1.50020200
H	-1.86357000	-2.35947400	-1.61488100
H	-3.06965400	-1.72582700	-2.25581000
O	-2.27197400	-0.63568700	-3.60632100
H	-2.59023100	-0.25069100	-4.43559600
H	-1.53062300	-1.25374900	-3.84801500
O	-2.16300200	3.31962300	-2.04821900
H	-1.75704000	3.88068900	-2.72558500
H	-1.93737300	3.76613600	-1.19202600
Gd	0.17435900	0.09317100	0.17999200

E = -1996.120215 Hartree

Zero-point correction =0.526972 Hartree/particle

Sum of electronic and thermal Energies =-1995.549678 Hartree

Sum of electronic and thermal Enthalpies = -1995.548864 Hartree

Sum of electronic and thermal Free Energies = -1995.671715 Hartree

Table S29: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, corresponding to Gd-O47(w) bond optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	3.08250900	-0.19292300	1.23942700
C	3.92839300	0.37936000	0.16595200
H	5.00022200	0.24687400	0.36803900
H	3.74035500	1.45911300	0.13595400
C	3.38436800	-1.64630400	1.46631900
C	2.11418000	-2.28971300	2.05973600
O	1.03601500	-2.07126400	1.39366000
O	2.17822700	-2.97158200	3.10510100
N	1.49464800	2.02996500	1.67384800
C	2.66282900	1.96850400	2.33357700
C	-0.49453000	3.16189400	0.92921200
O	-0.99578200	1.98034900	0.82694500
O	-1.04763100	4.22052000	0.56162600
O	-0.11448800	-1.71161400	-1.37392800
N	2.29583400	-0.61345600	-1.31851100
C	3.57488300	-0.22855400	-1.16960600
C	3.25957100	0.59038200	2.48066600
H	2.73027500	0.06425500	3.28402100

H	4.31408800	0.67080900	2.77473300
C	3.25914300	3.10590700	2.89028900
C	2.62622200	4.34137400	2.74832100
C	1.40578900	4.40249100	2.07411600
C	0.86901100	3.21832700	1.57030800
C	4.52297000	-0.40711100	-2.18374700
C	4.12515400	-0.99048900	-3.38680300
C	2.80252200	-1.41339100	-3.52996900
C	1.92699500	-1.22093600	-2.46237700
C	0.50261300	-1.71411900	-2.49930200
O	0.02277200	-2.07430900	-3.60062000
H	5.55118200	-0.10107200	-2.02347600
H	4.84093800	-1.13355600	-4.18962900
H	2.44120300	-1.89675300	-4.42955000
H	4.20332800	3.01837800	3.41684300
H	3.07609500	5.23870500	3.16035100
H	0.86161900	5.32991600	1.94140500
O	-0.78619500	0.87540200	-1.60247000
H	-1.30183600	0.29212300	-2.21100300
H	-1.32656800	1.70889800	-1.52044700
O	-0.34753600	-0.13620500	2.74601600
H	-0.38210500	-1.02069100	3.20887100
H	-1.18325000	0.36307200	2.96774700
H	3.48557400	-2.07993500	0.46599700
C	4.65228000	-1.94582700	2.26760400
H	4.83972200	-3.02198200	2.24130100
H	5.52524800	-1.44197800	1.84026400
H	4.55042400	-1.65510000	3.31578600
O	-2.73749700	-1.70749400	0.95881200
H	-2.90304500	-2.09139300	0.06614200
H	-3.51676700	-1.16754200	1.18594900
O	-0.32402100	-2.49531200	4.06468100
H	-0.16006600	-2.29209500	4.99765700
H	0.55204400	-2.82144300	3.72357200
O	-2.54637600	1.38113400	3.02453500
H	-2.24280400	1.75393100	2.16961700
H	-3.36145200	0.88371300	2.79153500
O	-4.76229700	-0.05048000	2.09428700
H	-5.31436900	-0.52153900	2.73629800
H	-5.37854900	0.49223000	1.58011000
O	-2.69982400	-2.80466200	-1.54711500
H	-1.73362000	-2.62185500	-1.49088500
H	-2.96653000	-2.11742800	-2.19037400
O	-2.27559400	-0.73389400	-3.33053800
H	-2.60467000	-0.31249900	-4.13765500
H	-1.51989100	-1.31907500	-3.60790900
O	-2.33253000	3.12178700	-1.59043200
H	-2.01700000	3.67775300	-2.31830400
H	-2.02283100	3.58945400	-0.77317700
Gd	0.36226800	-0.05090000	0.43259600

E = -1996.118593 Hartree

Zero-point correction =0.525138 Hartree/particle

Sum of electronic and thermal Energies =-1995.548325 Hartree

Sum of electronic and thermal Enthalpies = -1995.547381 Hartree

Sum of electronic and thermal Free Energies = -1995.670645 Hartree

Table S30: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, corresponding to Gd-O40(w) bond optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.34875000	-2.46773100	0.58622000
N	2.38404500	-1.37382700	0.03968900
C	0.88532200	-3.00599400	1.20829100
C	2.08816400	-2.80784100	0.28600900
C	-0.70009400	-3.25879300	-0.62462400
C	3.19864400	-0.80855700	1.13992100
C	-0.17939200	-2.65467400	-1.93802000
C	2.37666600	-0.28122300	2.32095200
O	-0.02298800	-3.40944900	-2.90982800
O	2.93293800	-0.11572500	3.41278500
O	1.14185100	0.03308000	2.05535200
O	0.01018000	-1.37739500	-1.92810500
C	3.08073300	-1.16981600	-1.25270700
C	3.00098800	0.31586500	-1.63639100
C	-1.48080700	-2.47745800	1.54304500
O	4.02623400	0.89831300	-2.05722400
O	1.85278000	0.87150600	-1.48384900
C	-2.65736300	-1.74371300	0.92866900
C	-3.99307400	-2.08419200	1.16829700
C	-4.99939700	-1.33295400	0.55634200
C	-4.64994000	-0.26309800	-0.27028000
C	-3.29490100	0.00858100	-0.46235400
N	-2.33027400	-0.72235300	0.12018300
H	-6.04259600	-1.58132100	0.72268600
H	-4.23505700	-2.92207800	1.81330500
H	-5.39104400	0.35822100	-0.75868200
C	-2.81725900	1.19727600	-1.27448800
O	-3.65796000	2.04149800	-1.64693300
O	-1.54264300	1.26911200	-1.46130100
H	1.03483200	-2.49185800	2.16017500
H	0.77596200	-4.08103500	1.41912700
H	2.96062400	-3.31575400	0.72200500
H	1.89350300	-3.28532300	-0.67808600

H	4.12753700	-1.49743000	-1.21853500
H	2.54895500	-1.74186100	-2.01827600
H	3.94651100	-1.52764900	1.49928200
H	3.74862900	0.05647500	0.75100300
H	-1.77202600	-3.49767300	1.82942500
H	-1.15781500	-1.95522900	2.45180200
O	1.37441400	3.15445100	0.44637900
H	0.70907700	3.43376500	-0.22875200
H	2.24767200	3.18719800	-0.01830700
O	-1.20407700	1.50475900	1.50134000
H	-0.61192500	1.99693500	2.13767200
H	-1.94046900	2.12130000	1.26276900
H	-1.79007800	-3.29234400	-0.71777700
H	-0.35594100	-4.29583100	-0.52869400
O	3.77637300	3.35329700	-0.89697500
H	4.49420700	3.27196800	-0.25201700
H	3.84459200	2.52031000	-1.43484400
O	0.69937400	2.63759900	2.98915800
H	1.02924800	1.71414100	3.00935600
H	1.05522500	2.96192400	2.12041300
O	-3.27258400	3.23699700	0.90675900
H	-3.56092800	3.02843900	-0.00664100
H	-4.02426900	2.97991600	1.46134700
O	-0.49021500	3.78890100	-1.48173800
H	-0.92974300	2.90938600	-1.59901500
H	-0.02459500	3.94492900	-2.31633200
Gd	0.11145900	0.09187700	-0.09164000

E = -1841.785306 Hartree

Zero-point correction =0.457987 Hartree/particle

Sum of electronic and thermal Energies =-1841.288869 Hartree

Sum of electronic and thermal Enthalpies = -1841.287925 Hartree

Sum of electronic and thermal Free Energies = -1841.397226 Hartree

Table S31: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, corresponding to Gd-O43(w) bond optimized at TPSSh/LCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.24500500	-2.45498300	0.53957000
N	2.50789000	-1.43486100	-0.01320300
C	0.97570200	-3.02882000	1.15303800
C	2.18105000	-2.86123500	0.23239600
C	-0.64487500	-3.24709500	-0.65414300
C	3.27565800	-0.86940300	1.12166200

C	-0.12586400	-2.68309100	-1.98612900
C	2.40114000	-0.34120100	2.26548300
O	-0.00337200	-3.45765000	-2.94543500
O	2.87983300	-0.24366900	3.39887100
O	1.20208900	0.04152800	1.92146400
O	0.09440100	-1.40797700	-2.00857800
C	3.27479600	-1.26798900	-1.27202700
C	3.21924700	0.21067800	-1.67654100
C	-1.35138800	-2.41877300	1.52305100
O	4.27324900	0.83200300	-1.94244000
O	2.04564700	0.73311000	-1.67712000
C	-2.51946800	-1.65003700	0.94369700
C	-3.85438500	-1.95957800	1.22765400
C	-4.86300600	-1.17356600	0.66779500
C	-4.51333100	-0.09674800	-0.14924300
C	-3.15978800	0.14208500	-0.38499300
N	-2.19083300	-0.62613000	0.13955300
H	-5.90573300	-1.39816200	0.86746600
H	-4.09233300	-2.80174200	1.86854800
H	-5.25360600	0.55426000	-0.59859300
C	-2.68930100	1.33200600	-1.19037100
O	-3.52116300	2.19710300	-1.53212000
O	-1.42093200	1.38325400	-1.43000800
H	1.14220100	-2.52665000	2.10875400
H	0.83796500	-4.10114400	1.36179600
H	3.04253100	-3.38850300	0.66800600
H	1.97435100	-3.33190200	-0.73264100
H	4.31424300	-1.60538600	-1.17374000
H	2.77606200	-1.85270200	-2.05002000
H	4.00444200	-1.59010200	1.51485900
H	3.84209100	-0.00516700	0.75467400
H	-1.66805600	-3.42611400	1.82830400
H	-0.98517200	-1.89832200	2.41617500
O	0.98676400	2.56818000	0.10556500
H	0.45733500	3.16809200	-0.49230600
H	1.93594500	2.70758300	-0.17966000
O	-1.80783700	1.63970200	2.04091700
H	-1.03440500	2.12085000	2.41628100
H	-2.41680100	2.33181700	1.70180300
H	-1.73703400	-3.23712900	-0.72968100
H	-0.34092000	-4.29616400	-0.55157000
O	3.51164700	3.14664800	-0.68523900
H	4.13078700	3.14815500	0.05946100
H	3.81476200	2.39409500	-1.25841400
O	0.64558400	2.61188600	2.84017300
H	0.88689500	1.65940700	2.83054400
H	0.81216100	2.83281200	1.89450800
O	-3.68404300	3.48900500	0.96793300
H	-3.74790800	3.15785700	0.04617400
H	-4.51199200	3.19973200	1.37915000

O	-0.53414100	3.91824500	-1.64300700
H	-0.99406700	3.04975000	-1.77416800
H	-0.02698500	4.05891100	-2.45644500
Gd	0.27581600	0.10108200	-0.24014300

E = -1841.780614 Hartree

Zero-point correction = 0.457826 Hartree/particle

Sum of electronic and thermal Energies = -1841.284112 Hartree

Sum of electronic and thermal Enthalpies = -1841.283168 Hartree

Sum of electronic and thermal Free Energies = -1841.393598 Hartree

Table S32: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, corresponding to Gd-O36(w) bond optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	2.87103100	-0.29148200	1.35675300
C	3.83972600	0.19465800	0.34408300
H	4.87569400	-0.04991700	0.61492200
H	3.76784600	1.28790600	0.31492000
C	3.06992000	-1.75432000	1.64267700
C	1.71805000	-2.30978700	2.13301200
O	0.71251600	-2.03261300	1.38393100
O	1.64894500	-2.97563400	3.19088300
N	1.41827400	2.02411600	1.52336400
C	2.49421600	1.93456900	2.32150300
C	-0.46041200	3.16566100	0.56274500
O	-0.92547200	1.98239900	0.37522800
O	-0.99607000	4.23415600	0.19591000
O	-0.25897700	-1.42496600	-1.44772000
N	2.21511200	-0.60962000	-1.25318600
C	3.51283400	-0.35042300	-1.02306800
C	2.99584300	0.53399200	2.58003400
H	2.35997800	0.08556700	3.35197800
H	4.02524100	0.56332400	2.95932600
C	3.05930500	3.06569300	2.92135600
C	2.48365300	4.31561400	2.68488500
C	1.34451500	4.39896200	1.88206900
C	0.83562300	3.22135600	1.33563200
C	4.49336200	-0.57434400	-1.99706300
C	4.10767500	-1.06347100	-3.24507700
C	2.76040600	-1.35054300	-3.47517900
C	1.85224700	-1.12513300	-2.44348900
C	0.39488800	-1.48923700	-2.55132900

O	-0.06505800	-1.83625900	-3.66212900
H	5.53529900	-0.37280800	-1.77318100
H	4.84929200	-1.23813800	-4.01761000
H	2.40508000	-1.75649200	-4.41456900
H	3.93216600	2.96376600	3.55706600
H	2.91155200	5.20767700	3.13062500
H	0.84124100	5.33783700	1.68432200
O	-0.75837200	1.32099500	-2.54745000
H	-1.40215200	0.68245800	-2.91209800
H	-1.32384200	2.07905700	-2.27714600
O	-0.19668200	0.16374100	2.75050500
H	-0.36161300	-0.66060000	3.27087000
H	-0.98254100	0.75492700	2.90496500
H	3.23316200	-2.21640400	0.66267100
C	4.24082900	-2.10122100	2.56188300
H	4.36030200	-3.18709400	2.58644500
H	5.17803200	-1.66748000	2.19944600
H	4.06470400	-1.76559800	3.58648200
O	-1.96897900	-0.65157800	0.60959500
H	-2.41661200	-1.15173500	-0.13177500
H	-2.33268000	-1.02211000	1.45259100
O	-0.71194100	-2.18627900	4.10875700
H	-0.56686600	-2.10261000	5.06236400
H	0.08961400	-2.66932200	3.74487000
O	-2.56641300	1.42933600	2.73933600
H	-2.43269900	1.50195700	1.77355300
H	-3.00555400	0.56255100	2.86098300
O	-3.01858700	-1.37208500	2.98556000
H	-2.28268500	-1.82567800	3.46733800
H	-3.75897900	-1.99407500	2.95048000
O	-2.86529000	-2.21370000	-1.35524900
H	-1.88815500	-2.27753000	-1.45888000
H	-3.08086300	-1.67283700	-2.14876400
O	-2.51175700	-0.72954600	-3.62141000
H	-2.93376200	-0.64871900	-4.48851600
H	-1.67897400	-1.25592100	-3.76505100
O	-2.46662800	3.51076400	-1.97889800
H	-2.14927700	4.16413300	-2.61950400
H	-2.04707000	3.79570300	-1.12630000
Gd	0.31865600	-0.02542800	0.40072300

E = -2725.557573 Hartree

Zero-point correction =0.527198 Hartree/particle

Sum of electronic and thermal Energies =-2724.986319 Hartree

Sum of electronic and thermal Enthalpies = -2724.985375 Hartree

Sum of electronic and thermal Free Energies = -2725.106814 Hartree

Table S33: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, corresponding to Gd-O39(w) bond optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	2.77720800	-0.20113000	1.22221700
C	3.75006600	0.28689200	0.21681300
H	4.78918500	0.07691900	0.50578200
H	3.64772200	1.37751300	0.16640500
C	2.92218800	-1.66756200	1.49782800
C	1.57766800	-2.14995200	2.07898600
O	0.53017700	-1.76771700	1.44461800
O	1.55825400	-2.87802100	3.09720200
N	1.28875900	2.08589400	1.52580400
C	2.40299100	1.98739900	2.26819300
C	-0.61448600	3.25011000	0.66058200
O	-1.08940400	2.07058300	0.46921100
O	-1.14414300	4.31835200	0.28240400
O	-0.23098200	-1.64332400	-1.46833600
N	2.17371800	-0.63810200	-1.35514700
C	3.45682800	-0.30705200	-1.13670200
C	2.92692800	0.58972800	2.46312300
H	2.30362400	0.12531500	3.23498700
H	3.96645100	0.61488500	2.81505500
C	2.98256900	3.10362400	2.88272800
C	2.38390600	4.35401200	2.72250200
C	1.21125800	4.45062400	1.97155800
C	0.69281000	3.28639300	1.40657900
C	4.45089500	-0.53490700	-2.09573200
C	4.09518200	-1.11679200	-3.31250300
C	2.76788000	-1.49936500	-3.51993500
C	1.84605300	-1.25912800	-2.50380000
C	0.41553500	-1.72220800	-2.57542500
O	-0.03927100	-2.13308000	-3.66856300
H	5.48059200	-0.26896100	-1.88252300
H	4.84679700	-1.29521900	-4.07445800
H	2.44025700	-1.99010500	-4.42841800
H	3.88533100	2.98748900	3.47279200
H	2.82096900	5.23438800	3.18246800
H	0.69136400	5.38976900	1.82428300
O	-0.58705500	0.97389100	-1.92257200
H	-1.16270200	0.41068600	-2.49376100
H	-1.04770600	1.85741400	-1.90989400
O	-0.01697500	0.40624500	3.51074700
H	-0.26165900	-0.48307400	3.83749400
H	-0.88107900	0.86009000	3.38048000
H	3.00069900	-2.14522300	0.51510800

C	4.12859600	-2.07356600	2.34577400
H	4.18748700	-3.16405900	2.37689800
H	5.06294300	-1.69702200	1.91775400
H	4.04013400	-1.71846800	3.37519300
O	-2.01038800	-0.61580700	0.50002000
H	-2.44721800	-1.15424600	-0.22129200
H	-2.29311400	-1.02465900	1.36036400
O	-0.77095800	-2.27892000	4.20847200
H	-0.74776900	-2.56124300	5.13302800
H	0.04621000	-2.65410200	3.76209000
O	-2.56487300	1.38012400	2.87300500
H	-2.31022300	1.51972100	1.93872100
H	-2.90282300	0.46092400	2.90103800
O	-2.89732900	-1.42455800	2.88820400
H	-2.16529600	-1.85515000	3.41044200
H	-3.64335100	-2.04018200	2.87982100
O	-2.88828800	-2.21722800	-1.43400600
H	-1.91206400	-2.33555200	-1.52061400
H	-3.05885200	-1.63459400	-2.20437900
O	-2.23346400	-0.59580200	-3.54694300
H	-2.53358000	-0.20016900	-4.37786100
H	-1.53649500	-1.26248400	-3.78557200
O	-1.97733900	3.31243900	-2.11702500
H	-1.48141300	3.89166600	-2.71455000
H	-1.85822700	3.72995400	-1.22605000
Gd	0.22514500	0.09103300	0.19169200

E = -2725.554928 Hartree

Zero-point correction = 0.527388 Hartree/particle

Sum of electronic and thermal Energies =-2724.983888 Hartree

Sum of electronic and thermal Enthalpies = -2724.982944 Hartree

Sum of electronic and thermal Free Energies = -2725.104848 Hartree

Table S34: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, corresponding to Gd-O47(w) bond optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	2.91378600	-0.13385700	1.22054500
C	3.82068600	0.33565400	0.14431800
H	4.87821900	0.16610000	0.38850700
H	3.68176600	1.41843300	0.04104000
C	3.12554800	-1.59328100	1.51633500
C	1.79248100	-2.13907900	2.05731500

O	0.75867000	-1.81932300	1.37131300
O	1.76703500	-2.84718900	3.09123300
N	1.40800200	2.15138700	1.54769900
C	2.53614400	2.06997600	2.26988600
C	-0.52298500	3.29141600	0.68560800
O	-0.95303800	2.11641600	0.41911200
O	-1.06940800	4.36778700	0.34755600
O	-0.32892000	-1.52473500	-1.32652800
N	2.16912900	-0.67476600	-1.29498400
C	3.46577000	-0.35073400	-1.15327900
C	3.10553700	0.68308900	2.43866300
H	2.55831500	0.19266400	3.25308800
H	4.15983100	0.74083400	2.73807200
C	3.09631500	3.19057700	2.89405600
C	2.45817800	4.42513500	2.76594900
C	1.27203000	4.50223100	2.03395900
C	0.77638300	3.33655900	1.45214400
C	4.41555600	-0.66868200	-2.13026900
C	4.00125200	-1.34103500	-3.28084000
C	2.65949600	-1.70480400	-3.40942600
C	1.77978600	-1.36189200	-2.38420800
C	0.32191400	-1.74551900	-2.41316800
O	-0.15615400	-2.21449800	-3.47156300
H	5.45665200	-0.40390900	-1.98119800
H	4.71870600	-1.59621800	-4.05378800
H	2.28506100	-2.24986300	-4.26738700
H	4.01308800	3.09120300	3.46512000
H	2.87812300	5.30974700	3.23360800
H	0.72680700	5.42988800	1.90726800
O	-0.23105900	1.10204900	-1.94345600
H	-0.87597900	0.58462800	-2.48116400
H	-0.61797100	2.01807300	-1.95117700
O	-0.54395100	0.22441400	2.50281500
H	-0.51977600	-0.61269200	3.02624600
H	-1.44320300	0.62350200	2.66716700
H	3.25302500	-2.07320200	0.54081200
C	4.33382400	-1.93235300	2.38973200
H	4.44903100	-3.01838700	2.42082500
H	5.25549900	-1.50738200	1.97963100
H	4.20793800	-1.58520200	3.41791100
O	-3.04959100	-0.66252600	0.73081100
H	-3.21563500	-1.12469300	-0.12853100
H	-3.08504800	-1.34742500	1.42903900
O	-0.59749500	-2.10740800	4.03013400
H	-0.41272400	-1.91893800	4.96155500
H	0.22391500	-2.55919500	3.66995400
O	-3.12973300	0.90013300	2.89672300
H	-3.28399400	0.65712100	1.95426100
H	-3.30769100	0.03471500	3.32533700
O	-3.16392200	-1.87717200	3.24343000

H	-2.26448200	-2.13198300	3.56470000
H	-3.77986500	-2.53139400	3.60034200
O	-3.06178700	-2.03534200	-1.59969700
H	-2.08332400	-2.06525200	-1.47805000
H	-3.12532100	-1.38299500	-2.32660300
O	-2.08302300	-0.31778200	-3.54043200
H	-2.28789900	0.08370800	-4.39729900
H	-1.49303000	-1.09020300	-3.73089000
O	-1.50540900	3.51739400	-2.21261400
H	-0.92245700	4.13368100	-2.68015700
H	-1.54095300	3.87710400	-1.29033200
Gd	0.33419100	0.15544200	0.28522100

E = -2725.549625 Hartree

Zero-point correction =0.527535 Hartree/particle

Sum of electronic and thermal Energies = -2724.978198 Hartree

Sum of electronic and thermal Enthalpies = -2724.977254 Hartree

Sum of electronic and thermal Free Energies = -2725.098641 Hartree

Table S35: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, corresponding to Gd-O43(w) bond optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.24826300	-2.55373600	0.46464800
N	2.47051100	-1.41634500	-0.00215100
C	0.98342600	-3.10122300	1.08345400
C	2.19972400	-2.86192400	0.19783100
C	-0.66268800	-3.37195000	-0.70524600
C	3.11257300	-0.81015100	1.19537200
C	-0.18330300	-2.81498500	-2.05449100
C	2.11468700	-0.17980300	2.18095600
O	-0.17291200	-3.57120300	-3.03499200
O	2.55417500	0.33050800	3.22736000
O	0.87721100	-0.16987500	1.81803600
O	0.13158200	-1.55918900	-2.06160100
C	3.31700400	-1.20058400	-1.20297000
C	3.16714300	0.25882200	-1.64685500
C	-1.33451500	-2.49620700	1.46970400
O	4.18163600	0.94906000	-1.89771800
O	1.95836500	0.68596300	-1.70499400
C	-2.50261300	-1.71302400	0.91644400
C	-3.83670500	-1.98310000	1.24108100
C	-4.83747600	-1.16130100	0.71925800
C	-4.48158900	-0.08899800	-0.10155800
C	-3.13083700	0.10455300	-0.38555900

N	-2.17042500	-0.69773100	0.10286300
H	-5.87949500	-1.35361500	0.95356000
H	-4.08022900	-2.81993400	1.88666400
H	-5.21509500	0.59128900	-0.51727700
C	-2.63549700	1.27498600	-1.20175700
O	-3.43288800	2.19035900	-1.49285900
O	-1.38112400	1.25377900	-1.50440300
H	1.11542000	-2.61372300	2.05123400
H	0.88000400	-4.18217500	1.26307400
H	3.07313100	-3.36393200	0.64000200
H	2.03471300	-3.30934200	-0.78610800
H	4.36910200	-1.45354200	-1.02432100
H	2.92661600	-1.83382200	-2.00490800
H	3.74765000	-1.53492800	1.72243100
H	3.77107100	0.00002600	0.86409700
H	-1.65529100	-3.49609600	1.79410400
H	-0.94101900	-1.96384400	2.34345500
O	0.85857400	2.34626500	0.20119400
H	0.27080900	2.98120700	-0.29066900
H	1.76475500	2.58164500	-0.15189400
O	-1.72559400	1.68342500	2.00822400
H	-0.89879900	2.00005700	2.43277600
H	-2.15189600	2.48651000	1.64423700
H	-1.75666200	-3.38373100	-0.75349600
H	-0.33928600	-4.41477400	-0.59720100
O	3.21688500	3.24885700	-0.80161500
H	3.85586100	3.36141900	-0.08245000
H	3.58546600	2.49818600	-1.33910200
O	0.77436000	2.64524800	2.96829900
H	1.25203500	1.83052600	3.23305600
H	0.88721100	2.63945100	1.98878300
O	-3.24579800	3.81615900	0.80184200
H	-3.35628400	3.37576200	-0.06848800
H	-4.08454700	3.64135000	1.25377500
O	-0.58208100	3.85078000	-1.53507600
H	-0.99153600	2.98231600	-1.77355900
H	0.10361800	3.98786900	-2.20630400
Gd	0.23766400	-0.07375400	-0.36084500

E = -2571.207447 Hartree

Zero-point correction = 0.458374 Hartree/particle

Sum of electronic and thermal Energies = -2570.710493 Hartree

Sum of electronic and thermal Enthalpies = -2570.709549 Hartree

Sum of electronic and thermal Free Energies = -2570.821214 Hartree

Table S36: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, corresponding to Gd-O40(w) bond optimized at TPSSh/SCRECP/6-31G(d,p), aqueous solution (1 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.33604500	-2.43598500	0.74901100
N	2.30464900	-1.27107700	-0.00073700
C	0.94073900	-2.91729500	1.33227200
C	2.09768700	-2.70078500	0.35859900
C	-0.76292400	-3.31150800	-0.37550700
C	3.09631900	-0.55154400	1.03008100
C	-0.39879600	-2.75800100	-1.76129100
C	2.23443400	0.02568900	2.16403800
O	-0.40730600	-3.53826200	-2.72584700
O	2.80363300	0.58989200	3.11764500
O	0.95935400	-0.06521000	2.01232500
O	-0.14954800	-1.49298600	-1.80734400
C	2.96273600	-1.15426300	-1.32550200
C	2.77257500	0.25916900	-1.89030700
C	-1.39976500	-2.36217900	1.77890700
O	3.72836500	0.82568600	-2.46399700
O	1.60276600	0.76720600	-1.72055000
C	-2.60807500	-1.65879400	1.19458300
C	-3.93141000	-1.96291000	1.53132000
C	-4.96106800	-1.21627800	0.95286000
C	-4.64701800	-0.18160000	0.06858700
C	-3.30356400	0.05209500	-0.22422400
N	-2.31879300	-0.68229200	0.31956900
H	-5.99567400	-1.43693500	1.19507500
H	-4.14668400	-2.76682300	2.22687500
H	-5.40778000	0.44129900	-0.38643300
C	-2.83876400	1.20597600	-1.09002900
O	-3.66427100	2.09058000	-1.40259200
O	-1.58360000	1.21247700	-1.37277100
H	1.10928800	-2.37497900	2.26269300
H	0.87900200	-3.99120500	1.56643800
H	3.01533000	-3.12719500	0.78903200
H	1.89665900	-3.24663100	-0.56736800
H	4.03017300	-1.40308100	-1.28437200
H	2.46188000	-1.84499300	-2.01004400
H	3.89168500	-1.18470000	1.44674900
H	3.58795600	0.30371200	0.55413600
H	-1.67611000	-3.35300900	2.16521000
H	-1.00877000	-1.76819100	2.61354300
O	1.49789700	2.59281700	0.38370400
H	0.96744800	3.01741200	-0.33516000
H	2.42492700	2.69069000	0.04722400

O	-1.03582200	1.65591700	1.39055800
H	-0.40275200	1.97218000	2.08723800
H	-1.46359300	2.46491900	1.01604800
H	-1.85367800	-3.40388600	-0.35739800
H	-0.35996300	-4.32514500	-0.26076700
O	3.94074800	2.98990600	-0.81573800
H	4.72897800	2.75790500	-0.30368800
H	3.90945400	2.31562600	-1.53909500
O	0.89574700	2.76968100	3.01379500
H	1.43572700	1.99484100	3.28390900
H	1.22320200	2.92057800	2.09259400
O	-2.33274900	3.87364900	0.30638600
H	-2.84811600	3.44307400	-0.41238800
H	-3.00334200	4.11958600	0.96098600
O	0.27908400	3.18347800	-2.01722300
H	-0.56794200	2.69660500	-1.90954700
H	0.89780100	2.44952800	-2.22641300
Gd	0.05312500	0.02291200	-0.10324700

E = -2571.216702 Hartree

Zero-point correction = 0.460896 Hartree/particle

Sum of electronic and thermal Energies = -2570.718522 Hartree

Sum of electronic and thermal Enthalpies = -2570.717578 Hartree

Sum of electronic and thermal Free Energies = -2570.824669 Hartree

Table S37: Cartesian coordinates (Å) of [Gd(cbda)(H_2O)$_3$].6H_2O complex, optimized at TPSSh/SARC-ZORA/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	2.85851000	-0.22740300	1.27704100
C	3.80423200	0.26014500	0.24946000
H	4.85119100	0.06285900	0.52193800
H	3.69191800	1.34937900	0.19084800
C	3.04186800	-1.68782700	1.56125900
C	1.68982400	-2.23163700	2.06837500
O	0.68301700	-1.98482800	1.31180500
O	1.62158200	-2.87110000	3.14447100
N	1.37009900	2.10314300	1.53990700
C	2.48741800	1.99406100	2.27556900
C	-0.55441300	3.28476900	0.72354500
O	-1.08961400	2.12064200	0.61940000
O	-1.06159900	4.35571700	0.31965900

O	-0.22082500	-1.64928200	-1.51940800
N	2.21764400	-0.66378300	-1.32719000
C	3.50123700	-0.34088400	-1.10077600
C	2.99720900	0.59053100	2.49817200
H	2.38039500	0.12998200	3.27834000
H	4.03335100	0.62321800	2.86171500
C	3.09184300	3.11002700	2.86773700
C	2.51530100	4.36848400	2.68855500
C	1.33464300	4.47404700	1.95100400
C	0.78748300	3.30898500	1.41303400
C	4.49978700	-0.56250500	-2.05761100
C	4.14713700	-1.11877300	-3.28708700
C	2.81569500	-1.47445500	-3.51282000
C	1.88968900	-1.24661500	-2.49589400
C	0.44837000	-1.67114700	-2.61359300
O	0.00355900	-2.00278300	-3.73934500
H	5.53041900	-0.30771800	-1.83415200
H	4.90189800	-1.29208500	-4.04719000
H	2.48686000	-1.93295100	-4.43769000
H	3.99579300	2.98807000	3.45511800
H	2.97277100	5.24860100	3.12870400
H	0.82824900	5.42009100	1.80025800
O	-0.76642900	1.00100000	-1.85376200
H	-1.29570600	0.42129200	-2.45232400
H	-1.29141900	1.84493200	-1.78866600
O	-0.25552800	0.16936100	2.74892900
H	-0.43420900	-0.68059000	3.21794100
H	-1.02630900	0.76026800	2.95750300
H	3.18767400	-2.15651900	0.58224000
C	4.22341200	-2.04814200	2.46418400
H	4.33750200	-3.13486500	2.48437700
H	5.15695700	-1.61908900	2.08624900
H	4.06777800	-1.71221000	3.49200100
O	-2.12833300	-0.70116600	0.49389100
H	-2.50223300	-1.30357900	-0.21132100
H	-2.50723000	-0.99794400	1.35917600
O	-0.80051200	-2.23797900	4.03541700
H	-0.65528700	-2.13204000	4.98703400
H	0.03959200	-2.65250800	3.67174200
O	-2.60940500	1.48258600	2.95717400
H	-2.46604900	1.72372800	2.01994900
H	-3.04624900	0.60552000	2.93900100
O	-3.10246100	-1.31544800	2.93523500
H	-2.36132600	-1.78763100	3.38991300
H	-3.86871700	-1.90631800	2.95823700
O	-2.84635500	-2.34592600	-1.47831500
H	-1.86429300	-2.39821000	-1.57069600
H	-3.05243400	-1.74353300	-2.22558900
O	-2.28874900	-0.63485900	-3.54307700
H	-2.61812100	-0.25414100	-4.36985600

H	-1.53731900	-1.24085100	-3.78788900
O	-2.23401700	3.30655000	-1.90812400
H	-1.81430300	3.84659200	-2.59455200
H	-1.96827500	3.74707000	-1.05948000
Gd	0.17767100	0.04781600	0.28230200

E = -12776.596791 Hartree

Zero-point correction = 0.526044 Hartree/particle

Sum of electronic and thermal Energies = -12776.026084 Hartree

Sum of electronic and thermal Enthalpies = -12776.025140 Hartree

Sum of electronic and thermal Free Energies = -12776.147777 Hartree

Table S38: Cartesian coordinates (Å) of $[Gd(peada)(H_2O)_2]^-.4H_2O$ complex, optimized at TPSSh/SARC-ZORA/6-31G(d,p), aqueous solution (0 Imaginary Frequency).

Atoms	X	Y	Z
N	-0.33356800	-2.46543100	0.54037500
N	2.43049500	-1.38593300	0.05428800
C	0.88237600	-2.99301900	1.20227800
C	2.11554200	-2.80967300	0.32150700
C	-0.66241100	-3.26204400	-0.66842200
C	3.19022900	-0.76336800	1.16596500
C	-0.15659600	-2.64175400	-1.97968700
C	2.30178500	-0.03159500	2.18191400
O	0.01969400	-3.38447600	-2.95824000
O	2.84074900	0.60001200	3.11252000
O	1.03282800	-0.08147800	1.97348900
O	-0.00219000	-1.35931700	-1.96753200
C	3.16900600	-1.22683900	-1.21899900
C	3.08842400	0.23995100	-1.65957200
C	-1.47639200	-2.45904400	1.47852800
O	4.12837500	0.84360900	-2.01727600
O	1.92289700	0.77132200	-1.60333200
C	-2.64491300	-1.71957600	0.86111600
C	-3.98083600	-2.06263200	1.09995500
C	-4.99017600	-1.29176200	0.51910000
C	-4.64185800	-0.19506600	-0.27180400
C	-3.28657900	0.07286100	-0.46970900
N	-2.31781800	-0.68224000	0.07378700
H	-6.03296900	-1.54127200	0.68635200
H	-4.21972600	-2.91686500	1.72464500
H	-5.38371400	0.45068200	-0.72634000
C	-2.81496600	1.29533900	-1.22871400
O	-3.65117100	2.17164100	-1.53319700

O	-1.54471500	1.36738600	-1.44491600
H	1.00413200	-2.46222500	2.14818100
H	0.76750600	-4.06699100	1.42162300
H	2.97006800	-3.31519900	0.79665400
H	1.95186300	-3.30229400	-0.64111400
H	4.21604600	-1.54781100	-1.13959800
H	2.66676200	-1.83186600	-1.97938700
H	3.81176500	-1.50231500	1.69178800
H	3.87666100	-0.01820500	0.75125700
H	-1.77913100	-3.47588800	1.76951400
H	-1.15903500	-1.93428000	2.38762300
O	1.06789300	2.63067600	0.24448600
H	0.48723900	3.19973300	-0.32990500
H	1.98082100	2.75655200	-0.13733800
O	-1.20167600	1.40502200	1.63172300
H	-0.52939300	1.83173500	2.22390800
H	-1.88015200	2.09397100	1.43177800
H	-1.75165100	-3.32074800	-0.76556000
H	-0.29568100	-4.29222700	-0.57668800
O	3.54475400	3.18495000	-0.75531100
H	4.18614100	3.13266100	-0.03114600
H	3.77472000	2.41371200	-1.33971200
O	0.83195500	2.72068300	2.96998800
H	1.43494600	1.97778800	3.19670400
H	1.03907400	2.87645900	2.01693200
O	-3.20879000	3.26539900	1.07746300
H	-3.49047300	3.08382100	0.15640900
H	-3.95960600	2.97360700	1.61618500
O	-0.55090700	3.88393600	-1.53462300
H	-1.03009500	3.02495800	-1.66574400
H	-0.01596700	3.99072100	-2.33567000
Gd	0.13694300	0.13208000	-0.17114700

E = -12622.251105 Hartree

Zero-point correction = 0.457961 Hartree/particle

Sum of electronic and thermal Energies = -12621.754059 Hartree

Sum of electronic and thermal Enthalpies = -12621.753115 Hartree

Sum of electronic and thermal Free Energies = -12621.865748 Hartree

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