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Supplementary Material

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Table S1 Variable temperature ^{17}O NMR relaxation rates and chemical shifts of $[Gd_3taci_2(H_2O)_6]^{3-}$ solution and of the reference at 14.1 T.

T/K	1000/T	P_m	T_1/s reference	T_1/s	$\ln(1/T_1r)$	T_2/s reference	T_2/s	$\ln(1/T_2r)$	ν (Hz) reference	ν (Hz)	$\Delta\omega_r$
315	3.17	2.96E-03	1.06E-02	8.96E-03	8.65	7.43E-03	1.06E-03	12.51	-116.6	-883.8	-1.63E+06
351	2.85	2.96E-03	2.03E-02	1.70E-02	8.10	1.37E-02	2.76E-03	11.49	-240.5	-924.9	-1.45E+06
365	2.74	2.96E-03	2.45E-02	2.05E-02	7.88	1.59E-02	3.83E-03	11.11	-308.7	-949	-1.36E+06
315	3.17	1.48E-03	1.06E-02	9.76E-03	8.57	7.43E-03	1.90E-03	12.49	-116.6	-488.6	-1.58E+06
351	2.85	1.48E-03	2.03E-02	1.84E-02	8.16	1.37E-02	5.07E-03	11.34	-260.5	-583.9	-1.37E+06
365	2.74	1.48E-03	2.45E-02	2.23E-02	7.89	1.59E-02	6.95E-03	10.91	-308.7	-593.2	-1.21E+06
303	3.30	1.48E-03	8.13E-03	7.54E-03	8.78	6.23E-03	1.39E-03	12.84	-78.1	-436.5	-1.52E+06
274	3.65	1.48E-03	3.45E-03	3.20E-03	9.64	2.92E-03	6.34E-04	13.64	27.6	-342.8	-1.57E+06
284	3.53	1.48E-03	4.69E-03	4.30E-03	9.46	3.84E-03	8.31E-04	13.37	-4.74	-387.4	-1.63E+06

Table S2 Variable temperature ^{17}O NMR relaxation rates and chemical shifts of $[Gd_3taci_2(H_2O)_6]^{3-}$ solution and of the reference at 9.4 T.

T/K	1000/T	P_m	T_1/s reference	T_1/s	$\ln(1/T_1r)$	T_2/s reference	T_2/s	$\ln(1/T_2r)$	ν (Hz) reference	ν (Hz)	$\Delta\omega_r$
272	3.68	2.96E-03	2.32E-03	1.96E-03		2.22E-03	2.84E-04	13.85	220.5	-212.7	-9.18E+05
321	3.12	2.96E-03	1.16E-02	9.75E-03	8.63	8.71E-03	1.32E-03	12.29	-1437.3	-1861.9	-9.00E+05
305	3.28	2.96E-03	8.80E-03	7.63E-03	8.69	7.02E-03	9.44E-04	12.64	-1392.1	-1881.6	-1.04E+06
343	2.91	2.96E-03	1.75E-02	1.47E-02	8.24	1.20E-02	2.32E-03	11.67	-1473.3	-1897.7	-8.99E+05
368	2.72	2.96E-03	2.42E-02	2.08E-02	7.71	1.66E-02	4.17E-03	11.01	-1529.4	-1928.1	-8.45E+05
290	3.45	2.96E-03	5.82E-03	4.92E-03	9.27	4.77E-03	5.17E-04	13.27	-1348	-1878.2	-1.12E+06
314	3.18	1.48E-03	1.02E-02	9.33E-03	8.72	7.65E-03	1.91E-03	12.49	-1406.8	-1640.7	-9.94E+05
281	3.56	1.48E-03	4.49E-03	4.12E-03	9.50	3.83E-03	8.05E-04	13.41	-1331.7	-1604.3	-1.16E+06
273	3.66	1.48E-03							-1314.8	-1566	-1.07E+06
347	2.89	1.48E-03				1.49E-02	4.21E-03	11.66	-124	-332.4	-8.86E+05
305	3.27	1.48E-03	8.60E-03	7.87E-03	8.90	6.08E-03	1.70E-03	12.57	-38.3	-280.9	-1.03E+06
275	3.64	1.48E-03	3.84E-03	3.51E-03	9.72	3.84E-03	7.28E-04	13.53	25.1	-223.1	-1.06E+06

Table S3 Variable temperature ^{17}O NMR relaxation rates and chemical shifts of $[Gd_3taci_2(H_2O)_6]^{3-}$ solution and of the reference at 1.41 T.

T/K	1000/T	P_m	T_2/s reference	T_2/s	ln(1/T_2r)	ν (Hz) reference	ν (Hz)	$\Delta\omega_r$
350.3	2.85	1.48E-03	1.67E-02	7.62E-03	10.78	60.8	37.9	-9.74E+04
306.1	3.27	1.48E-03	6.11E-03	3.76E-03	11.14			
321.4	3.11	1.48E-03	9.00E-03	5.19E-03	10.92	-1236.8	-1298	-2.60E+05
338.9	2.95	1.48E-03	1.73E-02	6.69E-03	11.04	-1499	-1532	-1.40E+05
352.4	2.84	1.48E-03	1.67E-02	9.50E-03		8.84	-9.15	-7.65E+04
366.6	2.73	1.48E-03	2.95E-02	1.00E-02	10.71	70.1	46.1	-1.02E+05
270.8	3.69	1.48E-03	2.69E-03	1.93E-03	11.50	-146	-185	-1.66E+05
289.9	3.45	1.48E-03	4.71E-03	2.85E-03	11.45	-41.9	-101	-2.51E+05

Table S4 Variable temperature ^{17}O NMR relaxation rates of $[Gd_3taci_2(H_2O)_6]^{3-}$ solution and of the reference at 0.572 T.

T/K	1000/T	P_m	T_2/s reference	T_2/s	ln(1/T_2r)
310.9	3.22	1.48E-03	6.68E-03	5.09E-03	10.36
330.6	3.02	1.48E-03	1.12E-02	7.43E-03	10.33
343.2	2.91	1.48E-03	1.47E-02	9.88E-03	10.02
272.7	3.67	1.48E-03	3.29E-03	2.87E-03	10.29
291.0	3.44	1.48E-03	4.36E-03	3.70E-03	10.22
362.7	2.76	1.48E-03	2.00E-02	1.34E-02	9.72

Table S5 Variable temperature transverse electronic relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution. B = 8.09 T, c_{Gd} = 0.06 M.

T/K	1000/T	ΔH_{pp} (Gauss)	$\ln(1/T_{2e})$
272.9	3.66	59.47	20.57
293.0	3.41	63.59	20.64
313.0	3.19	70.28	20.74
332.9	3.00	77.88	20.84
352.9	2.83	88.89	20.97
363.0	2.75	93.98	21.03
343.0	2.92	82.61	20.90
322.9	3.10	73.49	20.78
302.7	3.30	66.81	20.69
283.0	3.53	61.91	20.61

Table S6 Variable temperature transverse electronic relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution. B = 8.09 T, c_{Gd} = 0.04 M.

T/K	1000/T	ΔH_{pp} (Gauss)	$\ln(1/T_{2e})$
293.0	3.41	63.64	20.64
313.0	3.19	69.16	20.72
333.0	3.00	77.73	20.84
353.0	2.83	87.58	20.96
363.0	2.75	93.01	21.02
342.9	2.92	81.64	20.89
322.9	3.10	73.11	20.78
303.1	3.30	65.53	20.67
272.9	3.66	55.38	20.50

Table S7 Variable temperature transverse electronic relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution. B = 8.09 T, c_{Gd} = 0.02 M.

T/K	1000/T	ΔH_{pp} (Gauss)	$\ln(1/T_{2e})$
293.0	3.41	63.03	20.63
313.0	3.19	70.25	20.74
333.0	3.00	79.79	20.87
353.0	2.83	97.18	21.06
343.0	2.92	79.83	20.87
322.9	3.10	80.90	20.88
302.9	3.30	65.95	20.68
272.9	3.66	52.79	20.45

Table S8 Variable temperature transverse electronic relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution. B = 8.09 T, c_{Gd} = 0.009 M.

T/K	1000/T	ΔH_{pp} (Gauss)	$\ln(1/T_{2e})$
273.0	3.66	56.71	20.52
293.1	3.41	63.62	20.64
313.0	3.19	72.52	20.77
353.0	2.83	87.13	20.95
353.0	2.83	87.14	20.95
323.0	3.10	73.91	20.79
343.0	2.92	84.86	20.93
303.0	3.30	64.86	20.66
293.0	3.41	65.02	20.66
295.0	3.39	63.20	20.63
323.0	3.10	72.09	20.76
363.0	2.75	96.52	21.06

Table S9 Variable temperature transverse electronic relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution. B =2.7 T, c_{Gd} = 0.06 M.

T/K	1000/T	ΔH_{pp} (Gauss)	$\ln(1/T_{2e})$
293.0	3.41	122.60	21.40
293.0	3.41	128.17	21.44
313.0	3.19	135.31	21.50
273.0	3.66	113.76	21.32

Table S10 Variable temperature transverse electronic relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution. B =0.34 T, c_{Gd} = 0.06 M.

T/K	1000/T	ΔH_{pp} (Gauss)	$\ln(1/T_{2e})$
310.9	3.22	320.00	22.36
327.8	3.05	330.30	22.39
348.2	2.87	338.90	22.42
338.5	2.95	351.70	22.45
276.8	3.61	321.70	22.36
294.5	3.40	321.70	22.36
308.0	3.25	293.00	22.27
328.0	3.05	343.00	22.43
348.0	2.87	336.00	22.41
362.0	2.76	371.00	22.51

Table S11 Proton relaxivities (r_1 ; $mM^{-1}s^{-1}$) of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution.

ν (MHz)	25 °C	50 °C
9.998	6.511	4.916
7.998	6.857	5.045
6.398	7.307	5.407
5.117	7.691	5.919
4.095	8.337	5.670
3.276	8.507	6.130
2.622	8.899	6.092
2.098	9.167	6.224
1.679	9.443	6.437
1.342	9.510	6.389
1.074	9.690	6.335
0.859	9.815	6.482
0.687	9.847	6.449
0.550	9.927	6.433
0.440	9.868	6.680
0.352	9.962	6.556
0.282	9.885	6.679
0.225	9.932	6.486
0.180	9.827	6.745
0.144	9.956	6.685
0.115	9.904	6.381
0.092	9.967	6.520
0.074	9.878	6.574
0.059	9.972	6.463
0.047	10.008	6.404
0.038	9.935	6.481
0.030	9.992	6.364
12.001	6.417	4.596
14.999	5.881	4.391
16.000	5.643	4.323
18.002	5.611	4.219
20.001	5.482	4.139

Table S12 Variable pressure ^{17}O NMR relaxation rates of a $[Gd_3taci_2(H_2O)_6]^{3-}$ solution at 9.4T. (T= 355.8 K ; $P_m = 2.148 \times 10^{-3}$)

p / MPa	T2 / s	$\ln(1/T_{2r})$
0.6	3.78E-03	12.28
49	4.28E-03	12.11
100	4.66E-03	11.99
150	5.12E-03	11.84
194	5.25E-03	11.80
125	4.74E-03	11.96
77	4.33E-03	12.09
31	4.16E-03	12.15
0.6	4.01E-03	12.20