Electronic Supplementary Material (ESI) for RSC Advances

^{17}O and ^{1}H Relaxometric and DFT Study of Hyperfine Coupling Constants in $[Mn(H_2O)_6]^{2+}$

David Esteban-Gómez,[a] Claudio Cassino,[b] Mauro Botta[b] and Carlos Platas-Iglesias[a,*]

Supporting Information

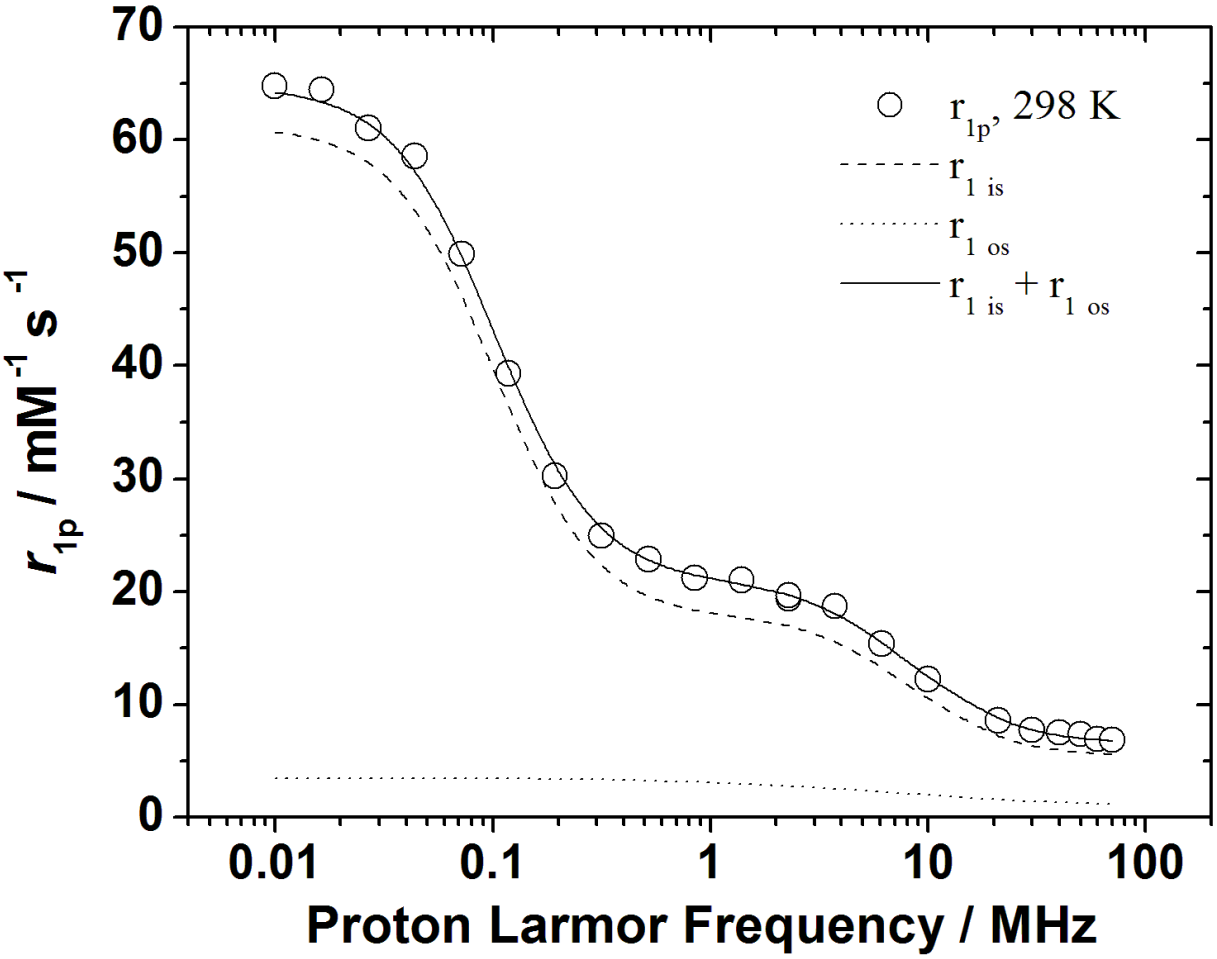

Fig. S1 ^{1}H NMRD profile recorded at 298 K for $[Mn(H_2O)_6]^{2+}$ (pH 1.7) and the calculated inner- and outer-sphere contributions to relaxivity obtained from the simultaneous fit of the NMRD and ^{17}O NMR data.

$[Mn(H_2O)_6]^{2+}$, TPSSh/svp (gas-phase, 0 imaginary frequencies)

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	25	0	0.000003	0.000006	-0.000011
2	8	0	1.365575	1.309772	1.110664
3	1	0	1.486267	2.268315	0.990994
4	8	0	-0.690330	1.717179	-1.177190
5	1	0	-1.431911	2.311720	-0.966805
6	8	0	1.574585	-0.383250	-1.479309
7	1	0	1.512528	-0.948271	-2.269602
8	8	0	0.690314	-1.717139	1.177226
9	1	0	0.317885	-2.041558	2.016103
10	8	0	-1.574575	0.383180	1.479323
11	1	0	-2.478136	0.020954	1.480592
12	8	0	-1.365572	-1.309757	-1.110689
13	1	0	-1.974475	-1.051341	-1.824920
14	1	0	1.974482	1.051354	1.824891
15	1	0	1.431889	-2.311698	0.966874
16	1	0	-1.512540	0.948211	2.269610
17	1	0	-0.317922	2.041631	-2.016064
18	1	0	2.478153	-0.021042	-1.480586
19	1	0	-1.486264	-2.268300	-0.991018

E(UTPSSh) = -1608.6657762 Hartree
Zero-point correction = 0.146577
Thermal correction to Energy = 0.165321
Thermal correction to Enthalpy = 0.166265
Thermal correction to Gibbs Free Energy = 0.099399
Sum of electronic and zero-point Energies = -1608.519200
Sum of electronic and thermal Energies = -1608.500455
Sum of electronic and thermal Enthalpies = -1608.499511
Sum of electronic and thermal Free Energies = -1608.566377

$[Mn(H_2O)_6]^{2+}\cdot 12H_2O$, TPSSh/svp (aqueous solution, 0 imaginary frequencies)

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	25	0	0.000024	0.000019	0.000229
2	8	0	1.698857	-0.634943	-1.273256
3	1	0	2.478381	-0.079244	-1.012087
4	8	0	-0.288905	1.771637	-1.298211
5	1	0	0.361315	2.457601	-0.993386
6	8	0	-1.389329	-1.148331	-1.291407
7	1	0	-2.310095	-0.922928	-0.996882
8	8	0	0.288943	-1.771546	1.298778
9	1	0	1.160605	-2.173503	1.048686
10	8	0	1.389444	1.148501	1.291797
11	1	0	1.303892	2.101126	1.026933
12	8	0	-1.698876	0.634864	1.273778
13	1	0	-2.478364	0.079105	1.012637
14	1	0	1.963804	-1.541133	-0.964032
15	1	0	-0.361264	-2.457518	0.993997
16	1	0	2.310260	0.923233	0.997334

17	1	0	-1.160549	2.173604	-1.048077
18	1	0	-1.303781	-2.100944	-1.026478
19	1	0	-1.963942	1.541037	0.964658
20	8	0	-2.420009	2.847098	-0.060555
21	8	0	-3.684118	-0.674433	0.023756
22	8	0	-1.256315	-3.516553	-0.032163
23	8	0	2.419781	-2.847243	0.061080
24	8	0	3.684186	0.674432	-0.023428
25	8	0	1.256218	3.516753	0.032588
26	1	0	-4.084412	-1.552930	0.212963
27	1	0	-4.377040	-0.003819	-0.170776
28	1	0	-2.182177	-3.781817	0.169425
29	1	0	-0.694355	-4.301715	-0.221868
30	1	0	2.184759	-3.776694	-0.159974
31	1	0	3.384971	-2.755736	0.229462
32	1	0	4.084345	1.552789	-0.213642
33	1	0	4.377232	0.003699	0.170187
34	1	0	0.694130	4.302076	0.221343
35	1	0	2.181849	3.782013	-0.169997
36	1	0	-3.385029	2.755562	-0.229919
37	1	0	-2.185081	3.776746	0.159661
38	8	0	3.988496	3.408371	-0.449954
39	8	0	-0.950707	5.150198	0.459115
40	8	0	-4.949509	1.760265	-0.433085
41	8	0	-3.988648	-3.408811	0.448975
42	8	0	0.950789	-5.149757	-0.460103
43	8	0	4.949689	-1.760566	0.432181
44	1	0	-1.042521	5.561637	1.336095
45	1	0	-1.074696	5.887624	-0.163442
46	1	0	-5.633621	2.018853	0.208639
47	1	0	-5.373253	1.894066	-1.298626
48	1	0	-4.562389	-3.888471	-0.173422
49	1	0	-4.299606	-3.693195	1.325952
50	1	0	1.042801	-5.561547	-1.336898
51	1	0	1.074647	-5.886940	0.162772
52	1	0	5.373089	-1.894130	1.297931
53	1	0	5.634050	-2.019368	-0.209187
54	1	0	4.562322	3.888184	0.172248
55	1	0	4.299207	3.692706	-1.327037

E(UTPSSh) =-2525.5477064 Hartree
Zero-point correction = 0.455780
Thermal correction to Energy = 0.500501
Thermal correction to Enthalpy = 0.501445
Thermal correction to Gibbs Free Energy = 0.378404
Sum of electronic and zero-point Energies = -2525.091926
Sum of electronic and thermal Energies = -2525.047206
Sum of electronic and thermal Enthalpies = -2525.046261
Sum of electronic and thermal Free Energies = -2525.169303