Hyperfine Coupling Constants on Inner-Sphere Water Molecules of a TACN-based Mn(II) Complex and Related Systems Relevant as MRI Contrast Agents

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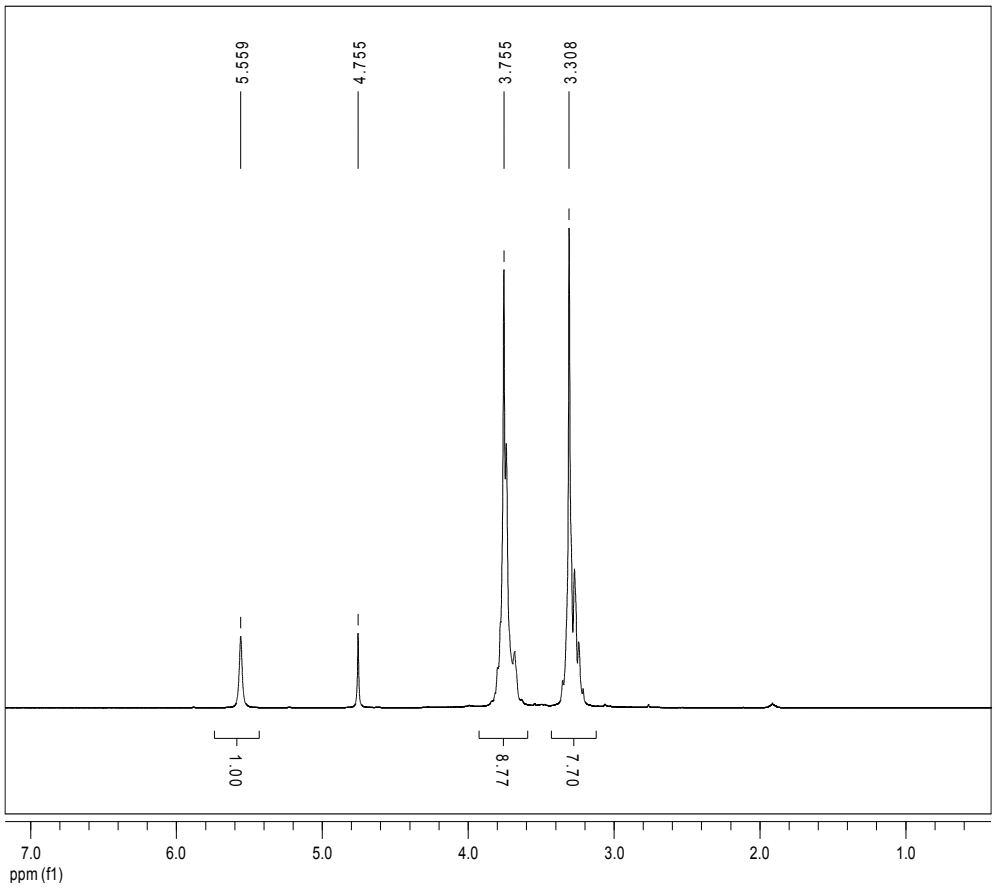
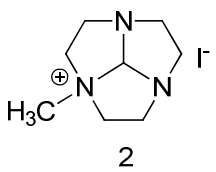
Supporting Information





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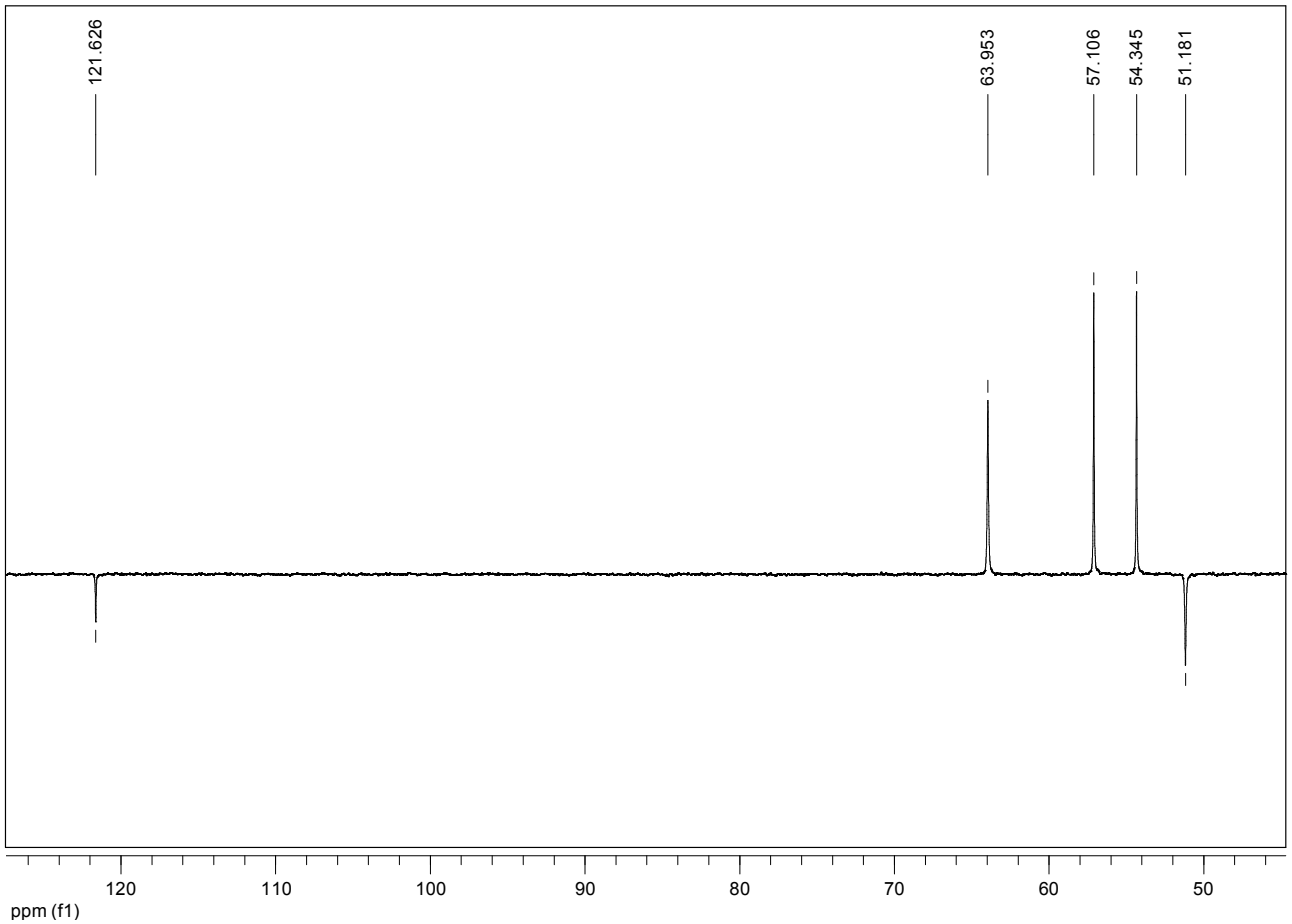
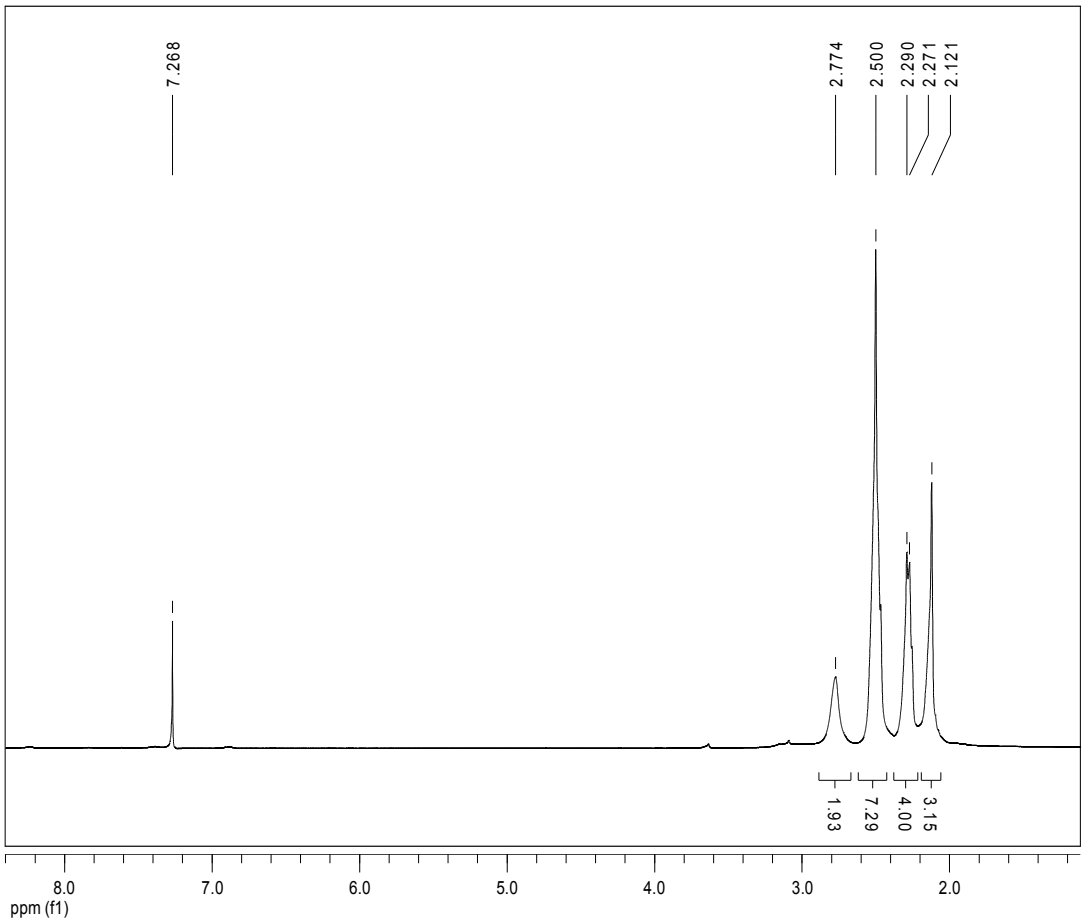
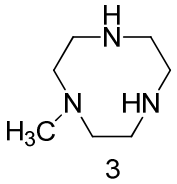


Figure S1. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of compound **2** (D_2O, 298K).





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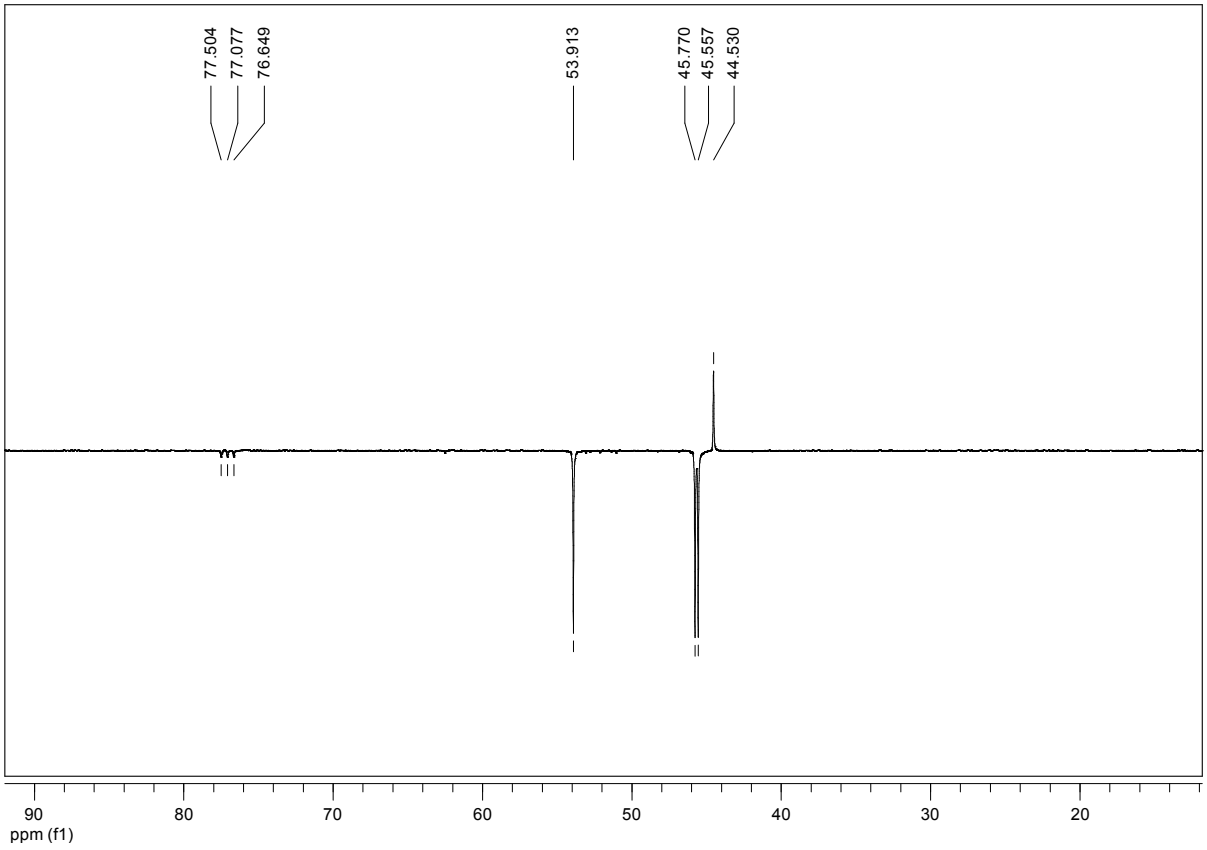
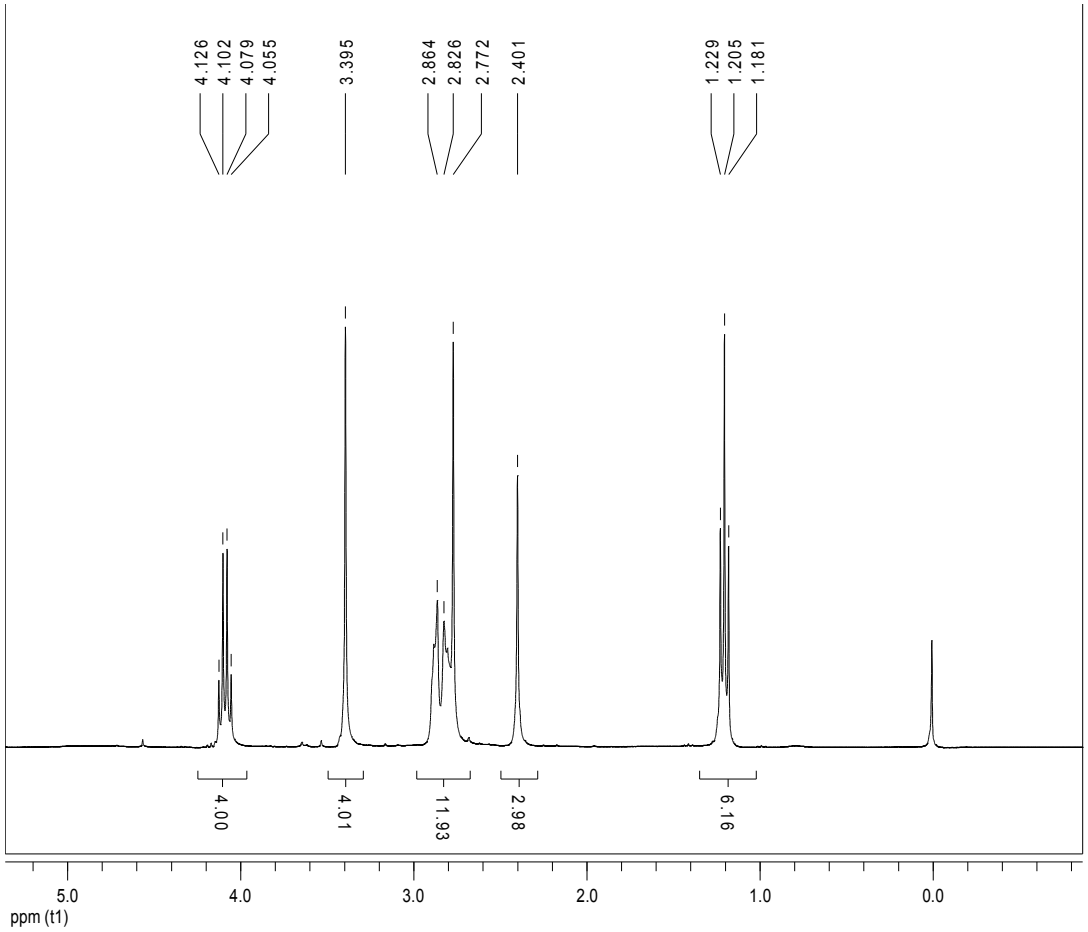
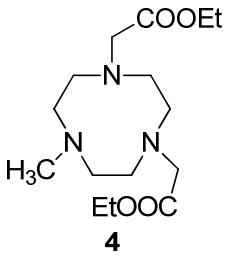


Figure S2. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of compound **3** ($CDCl_3$, 298K).





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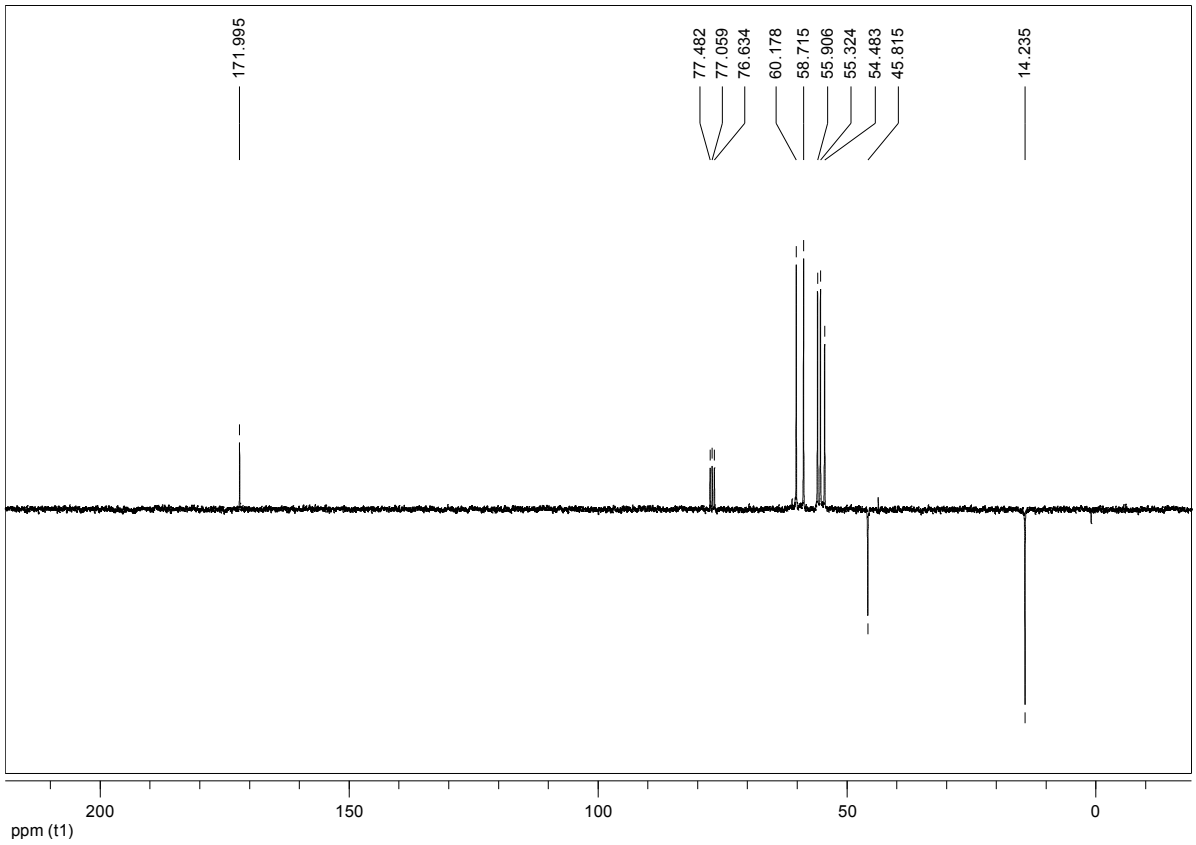
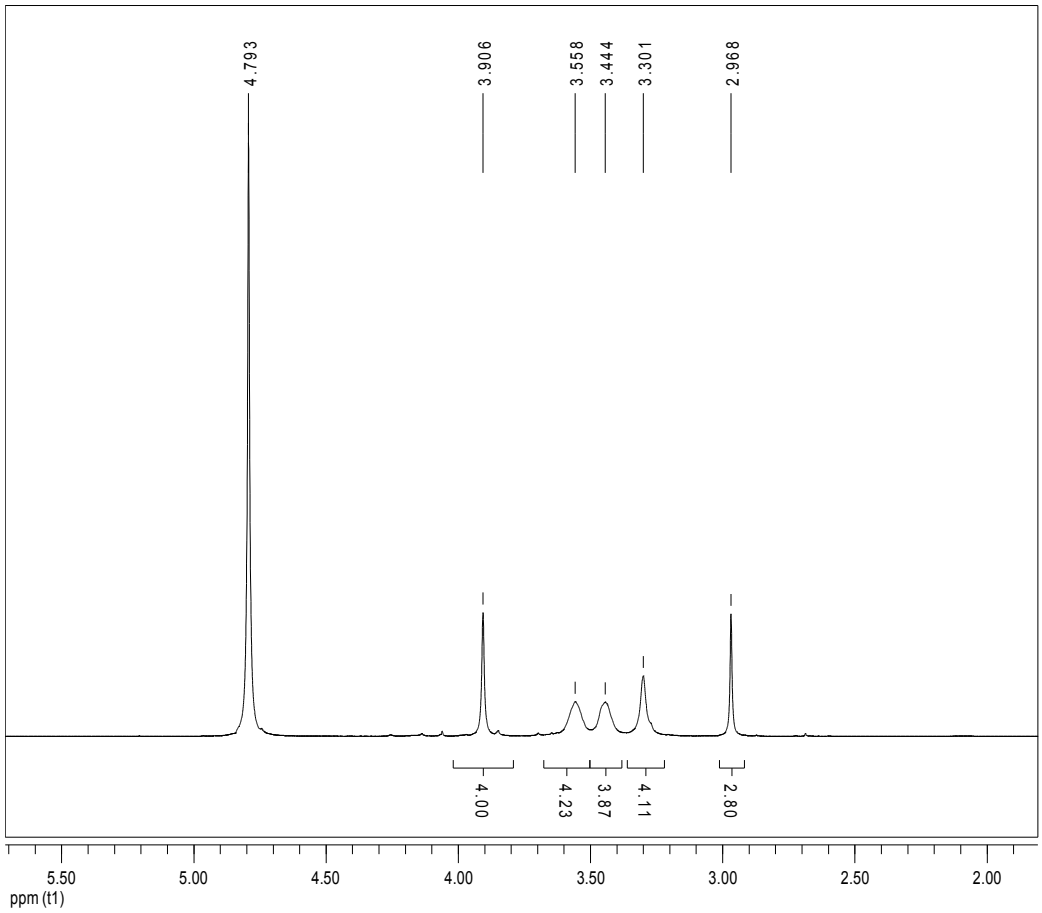
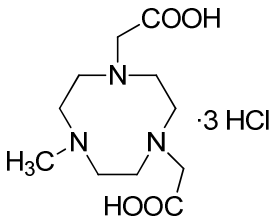


Figure S3. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of compound **4** ($CDCl_3$, 298K)





H_2MeNO2A·3HCl

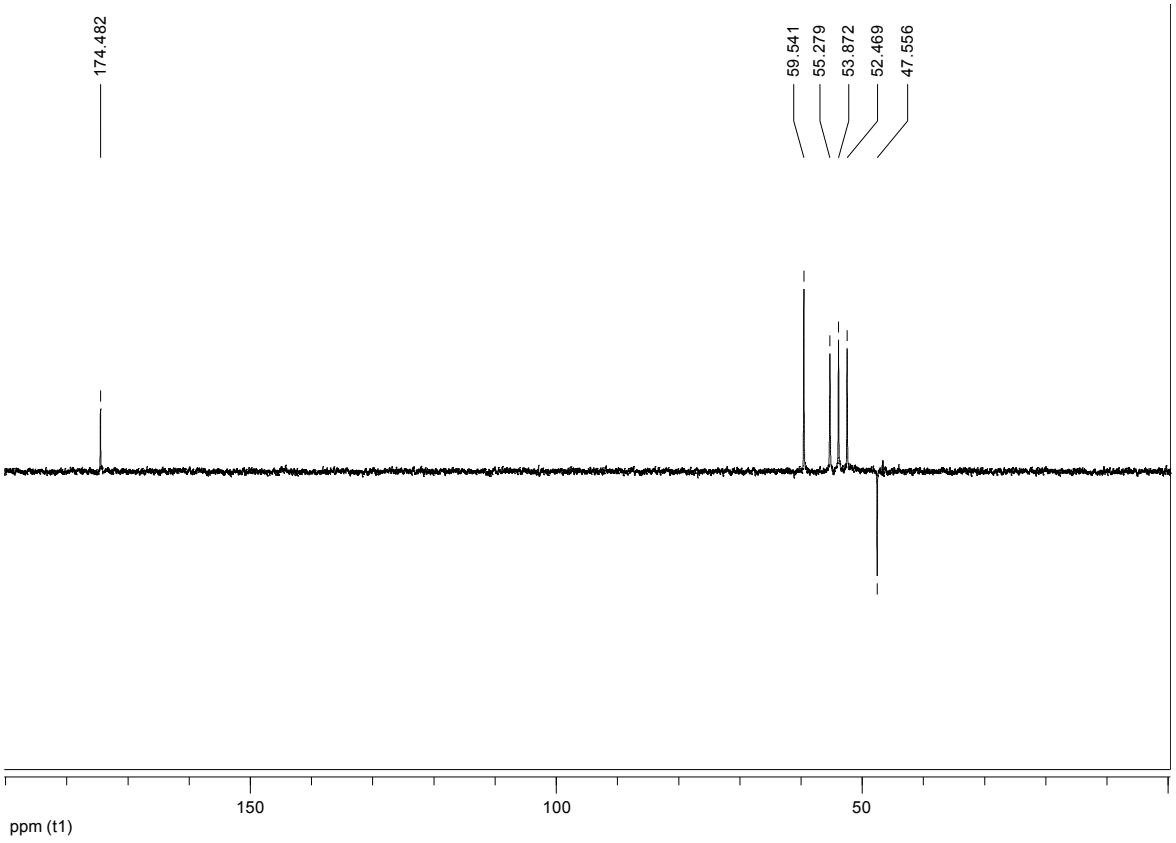


Figure S4. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of **H_2MeNO2A·3HCl** (D_2O, 298K).

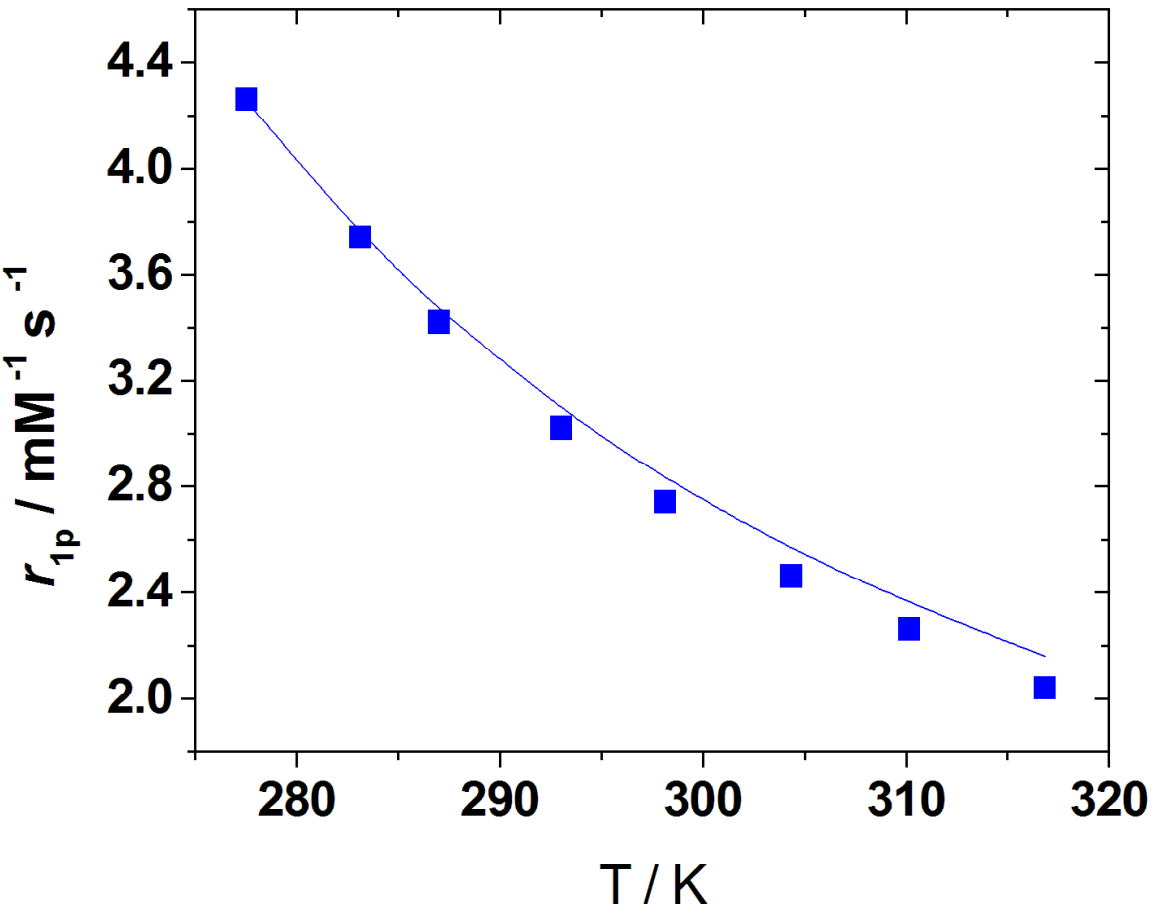


Figure S5. Temperature dependence of the proton relaxivity of [Mn(MeNO2A)] at 20 MHz and pH = 7.2. The solid line corresponds to the fit of the data with the parameters shown in Table 1.

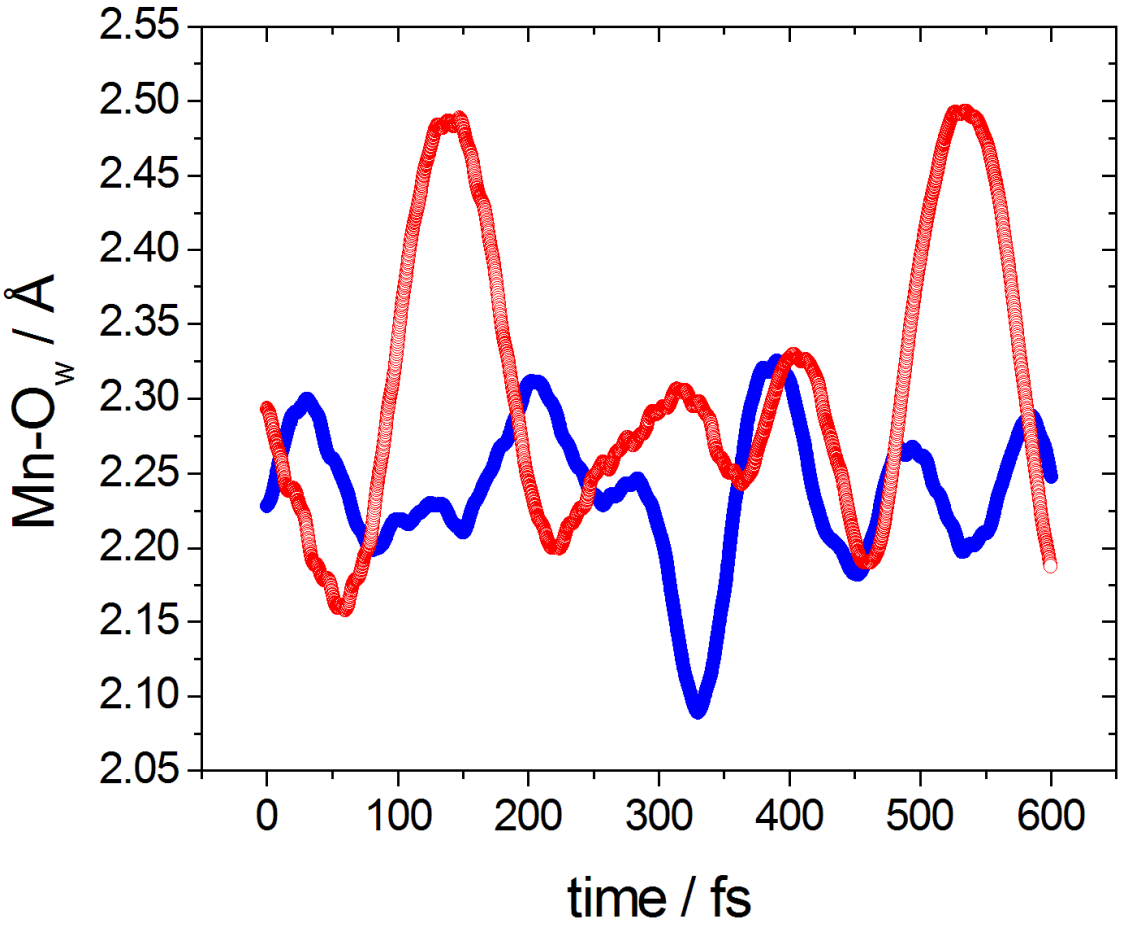


Figure S6. Calculated Mn-O distance during the full length of the ADMP simulations performed in aqueous solution on the [Mn(MeNO2A)(H_2O)]·4H_2O (●) and [Mn(MeNO2A)(H_2O)] (○) systems (TPSSh/SVP).

Equations used for the analysis of ^{17}O NMR and NMRD data

^{17}O NMR spectroscopy:

From the measured ^{17}O NMR transverse relaxation rates and angular frequencies of the paramagnetic solutions, $1/T_2$ and ω, and of the acidified water reference, $1/T_{2A}$ and ω_A, one can calculate the reduced relaxation rates, $1/T_{2r}$ and reduced chemical shifts (Eq. (1) – (2)), where $1/T_{2m}$ is the relaxation rate of the bound water and $\Delta\omega_m$ is the chemical shift difference between bound and bulk water, τ_m is the mean residence time or the inverse of the water exchange rate, k_{ex}, and P_m is the mole fraction of the bound water.[1,2]

$$\frac{1}{T_{2r}} = \frac{1}{P_m}\left[\frac{1}{T_2} - \frac{1}{T_{2A}}\right] = \frac{1}{\tau_m}\frac{T_{2m}^{-2} + \tau_m^{-1}T_{2m}^{-1} + \Delta\omega_m^2}{\left(\tau_m^{-1} + T_{2m}^{-1}\right)^2 + \Delta\omega_m^2} + \frac{1}{T_{2OS}} \qquad (1)$$

$$\Delta\omega_r = \frac{1}{P_m}(\omega - \omega_A) = \frac{\Delta\omega_m}{(1 + \tau_m T_{2m}^{-1})^2 + \tau_m^2\Delta\omega_m^2} + \Delta\omega_{os} \qquad (2)$$

The outer sphere contributions to the ^{17}O relaxation rates and chemical shifts have been considered to be negligible in the present study. $\Delta\omega_m$ is determined by the hyperfine or scalar coupling constant, $A/\hbar$, according to Equation (3), where B represents the magnetic field, S is the electron spin (S = 5/2 for high-spin Mn^{2+} complexes) and g_L is the isotropic Landé g factor.[3]

$$\Delta\omega_m = \frac{g_L\mu_B S(S+1)B}{3k_B T}\frac{A}{\hbar} \qquad (3)$$

The exchange rate is supposed to assume the Eyring equation. In Eq. (4) $\Delta S^{\ddagger}$ and $\Delta H^{\ddagger}$ are the entropy and enthalpy of activation for the water exchange process, and k_{ex}^{298} is the exchange rate at 298.15 K.

$$\frac{1}{\tau_m} = k_{ex} = \frac{k_B T}{h}\exp\left\{\frac{\Delta S^{\ddagger}}{R} - \frac{\Delta H^{\ddagger}}{RT}\right\} = \frac{k_{ex}^{298} T}{298.15}\exp\left\{\frac{\Delta H^{\ddagger}}{R}\left(\frac{1}{298.15} - \frac{1}{T}\right)\right\} \qquad (4)$$

In the transverse relaxation the scalar contribution, $1/T_{2sc}$, is the most important, Eq. (5). $1/\tau_{s1}$ is the sum of the exchange rate constant and the electron spin relaxation rate.

$$\frac{1}{T_{2m}} \cong \frac{1}{T_{2SC}} = \frac{S(S+1)}{3}\left(\frac{A}{\hbar}\right)^2 \tau_{S1} \tag{5}$$

$$\frac{1}{\tau_{S1}} = \frac{1}{\tau_m} + \frac{1}{T_{1e}} \tag{6}$$

^{1}H NMRD

The measured longitudinal proton relaxation rate, R_1^{obs} is the sum of a paramagnetic and a diamagnetic contribution as expressed in Eq. (7), where r_{1p} is the proton relaxivity:

$$R_1^{obs} = R_1^d + R_1^p = R_1^d + r_{1p}[Mn(II)] \tag{7}$$

The relaxivity can be divided into an inner and an outer sphere term as follows:

$$r_1 = r_{1is} + r_{1os} \tag{8}$$

The inner sphere term is given in Eq. (9), where q is the number of inner sphere water molecules.[4]

$$r_{1is} = \frac{1}{1000} \times \frac{q}{55.55} \times \frac{1}{T_{1m}^H + \tau_m} \tag{9}$$

The longitudinal relaxation rate of inner sphere protons, $1/T_{1m}{}^{H}$ is expressed by Eq. (10):

$$\frac{1}{T_{1m}^H} = \frac{2}{15}\left(\frac{\mu_0}{4\pi}\right)^2 \frac{\gamma_I^2 g^2 \mu_B^2}{r_{MnH}^6} S(S+1)\left[\frac{3\tau_{d1}}{1+\omega_I^2\tau_{d1}^2} + \frac{7\tau_{d2}}{1+\omega_S^2\tau_{d2}^2}\right] \tag{10}$$

where r_{MnH} is the effective distance between the electron charge and the ^{1}H nucleus, ω_I is the proton resonance frequency and ω_S is the Larmor frequency of the Mn(II) electron spin.

$$\frac{1}{\tau_{di}} = \frac{1}{\tau_m} + \frac{1}{\tau_R} + \frac{1}{T_{ie}} \qquad i = 1\,,\,2 \tag{11}$$

The longitudinal and transverse electronic relaxation rates, $1/T_{1e}$ and $1/T_{2e}$ are expressed by Eqs. (12)-(14),[5] where τ_V is the electronic correlation time for the modulation of the zero-field-splitting interaction, E_V the corresponding activation energy and Δ^2 is the mean square zero-field-splitting energy. We assumed a simple exponential dependence of τ_V versus $1/T$ as written in Eq. (14).

$$\frac{1}{T_{1e}} = \frac{1}{25}\Delta^2 \tau_V \{4S(S+1)-3\}\left(\frac{1}{1+\omega_s^2\tau_v^2} + \frac{4}{1+4\omega_s^2\tau_v^2}\right) \quad (12)$$

$$\frac{1}{T_{2e}} = \left(\left(0.02\times\left(4S^2+4S-3\right)\times\tau_V\times\Delta^2\times\left(\left(\frac{5}{1+{\omega_s}^2{\tau_V}^2}\right)\right)\right)+\left(\frac{2}{1+4{\omega_s}^2{\tau_V}^2}\right)+3\right) \quad (13)$$

$$\tau_v = \tau_v^{298}\exp\left\{\frac{E_v}{R}\left(\frac{1}{T}-\frac{1}{298.15}\right)\right\} \quad (14)$$

The outer-sphere contribution can be described by Eq. (15) where N_A is the Avogadro constant, and J_{os} is its associated spectral density function.[6,7]

$$r_{1os} = \frac{32N_A\pi}{405}\left(\frac{\mu_0}{4\pi}\right)^2\frac{\hbar^2\gamma_S^2\gamma_I^2}{a_{MnH}D_{MnH}}S(S+1)[3J_{os}(\omega_I;T_{1e})+7J_{os}(\omega_I;T_{2e})] \quad (15)$$

$$J^{OS}(\omega,T_{je}) = \mathrm{Re}\left[\frac{1+\frac{1}{4}\left(i\omega\tau_{MnH}+\frac{\tau_{MnH}}{T_{je}}\right)^{1/2}}{1+\left(i\omega\tau_{MnH}+\frac{\tau_{MnH}}{T_{je}}\right)^{1/2}+\frac{4}{9}\left(i\omega\tau_{MnH}+\frac{\tau_{MnH}}{T_{je}}\right)+\frac{1}{9}\left(i\omega\tau_{MnH}+\frac{\tau_{MnH}}{T_{je}}\right)^{3/2}}\right] \quad (16)$$

where $j = 1,2$, $\tau_{MnH} = \frac{{a_{MnH}}^2}{D_{MnH}}$.

The diffusion coefficient for the diffusion of a water proton away from a Gd(III) complex, D_{GdH}, is assumed to obey an exponential law versus the inverse of the temperature, with an activation energy E_{GdH}, as given in Eq. (17). ${D_{GdH}}^{298}$ is the diffusion coefficient at 298.15 K.

$$D_{MnH} = D_{MnH}^{298}\exp\left\{\frac{E_{MnH}}{R}\left(\frac{1}{298.15}-\frac{1}{T}\right)\right\} \quad (17)$$

$[Mn(EDTA)(H_2O)]^{2-}$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.031222	-0.021683	-0.763507
2	8	1.874656	1.082465	-1.221701
3	8	3.169164	2.739299	-0.431676
4	8	2.575043	-3.186870	0.540393
5	8	0.979691	-1.992100	-0.491231
6	8	-0.937268	1.932353	-0.919018
7	8	-2.631961	3.290526	-0.357693
8	8	-1.758632	-1.226964	-1.318389
9	8	-3.136570	-2.797198	-0.496084
10	7	-1.633259	0.104728	1.031817
11	7	1.321651	0.139050	1.244642
12	6	-0.937986	0.526764	2.253096
13	1	-0.842207	1.622947	2.218792
14	1	-1.530155	0.299598	3.163226
15	6	0.449695	-0.098564	2.401956
16	1	0.346538	-1.188390	2.518900
17	1	0.907978	0.268732	3.343015
18	6	1.859362	1.495740	1.137623
19	1	1.059790	2.222158	1.352846
20	1	2.676109	1.692192	1.859761
21	6	2.367567	1.811548	-0.293154
22	6	2.364454	-0.884556	1.126580
23	1	3.208869	-0.467862	0.556202
24	1	2.770824	-1.185438	2.110037
25	6	1.936020	-2.148897	0.347980
26	6	-2.614086	1.096336	0.581940
27	1	-3.360595	0.595406	-0.053677
28	1	-3.171869	1.548111	1.423447
29	6	-2.011293	2.223724	-0.290551
30	6	-2.168353	-1.255608	1.049714
31	1	-1.442382	-1.926096	1.536714
32	1	-3.113256	-1.339384	1.621707
33	6	-2.392572	-1.816342	-0.380231
34	8	1.048748	-0.769340	-2.949988
35	1	1.666589	-0.083268	-2.625755
36	1	1.205761	-1.501312	-2.319375

E(UB3LYP) = -2326.53833451 Hartree
Zero-point correction = 0.262218
Thermal correction to Energy = 0.284657
Thermal correction to Enthalpy = 0.285602
Thermal correction to Gibbs Free Energy = 0.208884
Sum of electronic and zero-point Energies = -2326.276116
Sum of electronic and thermal Energies = -2326.253677
Sum of electronic and thermal Enthalpies = -2326.252733
Sum of electronic and thermal Free Energies = -2326.329451

$[Mn(EDTA)(H_2O)]^{2-}\cdot H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.002720	-0.008566	-0.667231
2	8	2.122734	0.217044	-1.360613
3	8	3.912957	1.526279	-0.999202
4	8	1.526283	-3.554951	1.245172
5	8	0.300445	-2.097533	0.059096
6	8	-0.232208	2.094861	-1.127051
7	8	-1.391106	3.993728	-0.830478
8	8	-2.142529	-0.763190	-0.819517

9	8	-3.746261	-1.667349	0.465035
10	7	-1.337832	0.957873	1.112903
11	7	1.498197	0.075194	1.258529
12	6	-0.423463	1.395378	2.174891
13	1	0.009182	2.358378	1.863666
14	1	-0.962925	1.593996	3.123646
15	6	0.703786	0.399226	2.449864
16	1	0.273311	-0.540723	2.828301
17	1	1.337144	0.796035	3.269812
18	6	2.446176	1.108554	0.841608
19	1	1.963853	2.096157	0.913310
20	1	3.349079	1.146653	1.482961
21	6	2.887945	0.938388	-0.636904
22	6	2.124016	-1.246178	1.357048
23	1	3.011410	-1.270303	0.706289
24	1	2.482750	-1.466851	2.379748
25	6	1.239029	-2.414630	0.873100
26	6	-2.012228	2.089197	0.473163
27	1	-2.886262	1.710231	-0.079082
28	1	-2.391016	2.825837	1.207107
29	6	-1.132867	2.812863	-0.572926
30	6	-2.262401	-0.107381	1.491230
31	1	-1.740144	-0.834074	2.133145
32	1	-3.128339	0.262064	2.075611
33	6	-2.786371	-0.914312	0.279350
34	8	0.113387	-0.783296	-2.845806
35	1	1.081483	-0.829050	-2.759182
36	1	-0.240926	-1.701878	-2.710373
37	8	-1.157786	-2.996404	-2.011179
38	1	-1.797032	-2.303589	-1.718901
39	1	-0.565173	-2.980346	-1.221514

E(UB3LYP) = -2402.9337432 Hartree
Zero-point correction = 0.288336
Thermal correction to Energy = 0.312733
Thermal correction to Enthalpy = 0.313677
Thermal correction to Gibbs Free Energy = 0.233126
Sum of electronic and zero-point Energies = -2402.645407
Sum of electronic and thermal Energies = -2402.621010
Sum of electronic and thermal Enthalpies = -2402.620066
Sum of electronic and thermal Free Energies = -2402.700617

$[Mn(EDTA)(H_2O)]^{2-}\cdot 2H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.034661	0.079581	-0.556491
2	8	-2.227926	-0.555154	-0.685861
3	8	-3.649884	-2.174663	-0.055088
4	8	-1.487458	2.978566	2.269845
5	8	-0.502012	1.939132	0.543940
6	8	0.367133	-1.874080	-1.373515
7	8	1.777422	-3.593767	-1.667444
8	8	1.908207	1.217262	-0.986947
9	8	3.673459	2.171144	0.018753
10	7	1.868642	-0.891048	0.712985
11	7	-0.931780	-0.553529	1.670098
12	6	1.328647	-1.607067	1.873619
13	1	0.961208	-2.584301	1.525266
14	1	2.117044	-1.828140	2.622449
15	6	0.192867	-0.852824	2.563940
16	1	0.574707	0.104367	2.951275
17	1	-0.133757	-1.432328	3.452095
18	6	-1.779399	-1.703361	1.360204
19	1	-1.144034	-2.575758	1.141332

20	1	-2.440209	-1.990605	2.202168
21	6	-2.649980	-1.471720	0.105844
22	6	-1.703589	0.604316	2.130036
23	1	-2.728646	0.531334	1.735016
24	1	-1.797052	0.636755	3.231560
25	6	-1.176379	1.968655	1.633603
26	6	2.483485	-1.799527	-0.255297
27	1	3.132532	-1.213896	-0.925492
28	1	3.128161	-2.559166	0.227211
29	6	1.457717	-2.508989	-1.168964
30	6	2.727272	0.240122	1.047412
31	1	2.319706	0.760799	1.928317
32	1	3.757495	-0.066854	1.317143
33	6	2.800762	1.302126	-0.071948
34	8	-0.563280	1.110956	-2.504314
35	1	-1.541784	1.129437	-2.640166
36	1	-0.293181	2.043591	-2.310172
37	8	-3.292668	0.893505	-2.592782
38	1	-3.058059	0.227683	-1.885156
39	1	-3.592764	1.658065	-2.079218
40	8	0.462340	3.422515	-1.520172
41	1	1.230105	2.803879	-1.459588
42	1	0.005941	3.163924	-0.685357

E(UB3LYP) = -2479.3232002 Hartree
Zero-point correction = 0.313497
Thermal correction to Energy = 0.340476
Thermal correction to Enthalpy = 0.341420
Thermal correction to Gibbs Free Energy = 0.254546
Sum of electronic and zero-point Energies = -2479.009703
Sum of electronic and thermal Energies = -2478.982725
Sum of electronic and thermal Enthalpies = -2478.981780
Sum of electronic and thermal Free Energies = -2479.068654

$[Mn(EDTA)(H_2O)]^{2-}\cdot 3H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.048490	0.066646	0.363993
2	8	-2.285319	0.330656	0.048797
3	8	-3.808173	1.029921	-1.445302
4	8	-0.765223	-4.110214	-0.257270
5	8	-0.118000	-2.121196	0.552654
6	8	0.024896	2.201082	-0.072277
7	8	1.232848	3.988250	-0.685808
8	8	1.940398	-0.224524	1.447795
9	8	3.906863	-1.288069	1.246657
10	7	1.848647	0.454123	-1.169778
11	7	-0.745242	-0.840194	-1.821985
12	6	1.375102	0.270400	-2.546649
13	1	0.853959	1.191435	-2.849260
14	1	2.218905	0.150112	-3.256545
15	6	0.431658	-0.922731	-2.695954
16	1	0.971057	-1.848578	-2.443990
17	1	0.141982	-1.019454	-3.762327
18	6	-1.759887	0.111778	-2.271734
19	1	-1.266352	1.034551	-2.614467
20	1	-2.356208	-0.267039	-3.125069
21	6	-2.724343	0.529041	-1.141068
22	6	-1.306351	-2.162840	-1.529560
23	1	-2.368772	-2.048940	-1.263598
24	1	-1.276028	-2.835691	-2.406660
25	6	-0.661652	-2.883889	-0.324606
26	6	2.245372	1.837275	-0.901641
27	1	2.904958	1.850065	-0.019854
28	1	2.823931	2.281171	-1.733906

29	6	1.071103	2.774205	-0.548200
30	6	2.862107	-0.509636	-0.749475
31	1	2.611352	-1.502648	-1.153991
32	1	3.873106	-0.263800	-1.130291
33	6	2.934957	-0.685946	0.782612
34	8	-0.709801	0.299142	2.552040
35	1	-1.694779	0.222171	2.639795
36	1	-0.302283	-0.502542	2.973677
37	8	-3.410467	0.300010	2.412271
38	1	-3.161012	0.411265	1.450132
39	1	-3.739214	-0.610077	2.452226
40	8	0.712350	-1.899711	3.148920
41	1	1.405428	-1.313910	2.757773
42	1	0.355976	-2.276477	2.310995
43	8	-0.948996	3.121721	2.359404
44	1	-0.735711	2.990648	1.411997
45	1	-0.751261	2.231576	2.700490

E(UB3LYP) = -2555.7059902 Hartree
Zero-point correction = 0.338782
Thermal correction to Energy = 0.368235
Thermal correction to Enthalpy = 0.369179
Thermal correction to Gibbs Free Energy = 0.277349
Sum of electronic and zero-point Energies = -2555.367208
Sum of electronic and thermal Energies = -2555.337755
Sum of electronic and thermal Enthalpies = -2555.336811
Sum of electronic and thermal Free Energies = -2555.428641

$[Mn(EDTA)(H_2O)]^{2-}\cdot 4H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.088556	-0.124985	0.267837
2	8	1.904849	-1.456860	0.420334
3	8	3.395991	-2.627894	-0.781414
4	8	2.770534	3.130585	0.981955
5	8	1.062975	1.678092	1.043890
6	8	-0.844523	-1.849456	-0.706812
7	8	-2.360493	-2.638615	-2.158427
8	8	-1.816943	1.046866	0.923226
9	8	-2.841775	3.009927	0.556914
10	7	-1.143707	0.719942	-1.677007
11	7	1.802861	0.547997	-1.369934
12	6	-0.220221	0.784032	-2.817753
13	1	-0.116957	-0.233871	-3.223580
14	1	-0.631980	1.400939	-3.642017
15	6	1.156695	1.324621	-2.434969
16	1	1.055864	2.360690	-2.077665
17	1	1.788924	1.375469	-3.344653
18	6	2.361474	-0.729815	-1.809101
19	1	1.647217	-1.224931	-2.485645
20	1	3.308162	-0.614719	-2.372338
21	6	2.599076	-1.700875	-0.632830
22	6	2.766852	1.350211	-0.610146
23	1	3.503638	0.677408	-0.144485
24	1	3.340613	2.040890	-1.255331
25	6	2.154251	2.151173	0.559763
26	6	-2.203367	-0.270399	-1.882761
27	1	-3.001008	-0.097388	-1.144186
28	1	-2.654660	-0.206810	-2.890566
29	6	-1.766680	-1.717402	-1.597742
30	6	-1.673993	2.019010	-1.269538
31	1	-0.877410	2.776873	-1.328442
32	1	-2.489884	2.372682	-1.930197
33	6	-2.175147	2.043884	0.187710

34	8	-0.192484	-0.875849	2.433256
35	1	0.638337	-1.304086	2.771307
36	1	-0.314333	-0.021359	2.929121
37	8	2.123461	-2.157661	2.940081
38	1	2.183709	-2.051154	1.948185
39	1	2.772828	-1.521110	3.273832
40	8	-0.557701	1.656140	3.232431
41	1	-1.284220	1.577634	2.570751
42	1	0.178106	1.879154	2.614389
43	8	-1.884155	-2.915012	1.602493
44	1	-1.496535	-2.777703	0.708798
45	1	-1.380418	-2.246325	2.113381
46	8	-3.829234	-0.940197	1.130984
47	1	-3.188314	-0.202568	1.156460
48	1	-3.247312	-1.717838	1.278459

E(UB3LYP) = -2632.0973235 Hartree
Zero-point correction = 0.365215
Thermal correction to Energy = 0.396703
Thermal correction to Enthalpy = 0.397647
Thermal correction to Gibbs Free Energy = 0.301523
Sum of electronic and zero-point Energies = -2631.732109
Sum of electronic and thermal Energies = -2631.700621
Sum of electronic and thermal Enthalpies = -2631.699677
Sum of electronic and thermal Free Energies = -2631.795801

$[Mn(EDTA)(H_2O)]^{2-}$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.032895	-0.015322	-0.745817
2	8	1.880719	1.039779	-1.250758
3	8	3.176052	2.717608	-0.490115
4	8	2.521654	-3.212141	0.579721
5	8	0.910593	-2.018336	-0.441833
6	8	-0.891522	1.958514	-0.880289
7	8	-2.587633	3.321962	-0.312367
8	8	-1.774880	-1.175946	-1.331966
9	8	-3.149303	-2.761464	-0.516536
10	7	-1.607480	0.111519	1.019885
11	7	1.322222	0.140681	1.210852
12	6	-0.914010	0.538402	2.242292
13	1	-0.809906	1.633836	2.194034
14	1	-1.508305	0.319434	3.152078
15	6	0.467277	-0.099531	2.382395
16	1	0.357837	-1.190609	2.485894
17	1	0.941123	0.259404	3.317949
18	6	1.865275	1.497314	1.100907
19	1	1.063575	2.223471	1.310076
20	1	2.682480	1.691772	1.822676
21	6	2.373360	1.789672	-0.332783
22	6	2.367117	-0.882197	1.086395
23	1	3.175670	-0.475741	0.458772
24	1	2.815823	-1.144872	2.062407
25	6	1.895380	-2.165552	0.372241
26	6	-2.594578	1.102243	0.575439
27	1	-3.317153	0.598971	-0.085889
28	1	-3.170044	1.528636	1.418227
29	6	-1.975407	2.245375	-0.259531
30	6	-2.146645	-1.249521	1.041587
31	1	-1.407006	-1.920931	1.506714
32	1	-3.080430	-1.333035	1.631187
33	6	-2.396688	-1.783756	-0.392393
34	8	0.997445	-0.844486	-2.895944
35	1	1.641546	-0.169546	-2.588276

36	1	1.122490	-1.561742	-2.234172

E(UTPSSh) = -2326.5670796 Hartree
Zero-point correction = 0.260957
Thermal correction to Energy = 0.283571
Thermal correction to Enthalpy = 0.284516
Thermal correction to Gibbs Free Energy = 0.207505
Sum of electronic and zero-point Energies = -2326.306123
Sum of electronic and thermal Energies = -2326.283508
Sum of electronic and thermal Enthalpies = -2326.282564
Sum of electronic and thermal Free Energies = -2326.359575

$[Mn(EDTA)(H_2O)]^{2-}\cdot H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.003522	-0.004780	-0.639194
2	8	2.126092	0.136045	-1.340770
3	8	3.918027	1.460572	-1.003628
4	8	1.484040	-3.574484	1.228654
5	8	0.248371	-2.091534	0.073983
6	8	-0.145666	2.107591	-1.082024
7	8	-1.306224	4.016127	-0.809334
8	8	-2.141787	-0.727157	-0.843392
9	8	-3.766380	-1.632087	0.424764
10	7	-1.327761	0.957984	1.090374
11	7	1.474235	0.057612	1.250904
12	6	-0.421501	1.400255	2.159891
13	1	0.027502	2.351486	1.834091
14	1	-0.969043	1.615723	3.099265
15	6	0.684992	0.386147	2.446389
16	1	0.237076	-0.551378	2.811521
17	1	1.322987	0.768702	3.268476
18	6	2.434956	1.084162	0.837731
19	1	1.950028	2.071968	0.889127
20	1	3.328167	1.123255	1.492099
21	6	2.888396	0.881186	-0.630709
22	6	2.096546	-1.267715	1.353711
23	1	2.980101	-1.290359	0.697423
24	1	2.454323	-1.484440	2.377393
25	6	1.199644	-2.424972	0.872519
26	6	-1.991237	2.092482	0.440283
27	1	-2.835310	1.702432	-0.150365
28	1	-2.404330	2.815012	1.169585
29	6	-1.067328	2.826717	-0.556005
30	6	-2.269601	-0.094015	1.472204
31	1	-1.753334	-0.825223	2.114393
32	1	-3.130318	0.291465	2.053195
33	6	-2.795285	-0.884971	0.253541
34	8	0.107841	-0.741532	-2.832497
35	1	1.076514	-0.783505	-2.707963
36	1	-0.248768	-1.664213	-2.686308
37	8	-1.166697	-2.946502	-2.018948
38	1	-1.804427	-2.243498	-1.729748
39	1	-0.586867	-2.939092	-1.213072

E(UTPSSh) = -2402.9563341 Hartree
Zero-point correction = 0.286820
Thermal correction to Energy = 0.311344
Thermal correction to Enthalpy = 0.312288
Thermal correction to Gibbs Free Energy = 0.231513
Sum of electronic and zero-point Energies = -2402.669514
Sum of electronic and thermal Energies = -2402.644990
Sum of electronic and thermal Enthalpies = -2402.644046
Sum of electronic and thermal Free Energies = -2402.724821

$[Mn(EDTA)(H_2O)]^{2-}\cdot 2H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.024422	0.068533	-0.528140
2	8	-2.240529	-0.472263	-0.654627
3	8	-3.674384	-2.099421	-0.047381
4	8	-1.452184	3.023182	2.232190
5	8	-0.425569	1.946457	0.545960
6	8	0.273655	-1.925139	-1.294459
7	8	1.680558	-3.649999	-1.620624
8	8	1.922065	1.172267	-1.020980
9	8	3.695725	2.130332	-0.020465
10	7	1.842744	-0.898053	0.692210
11	7	-0.920203	-0.520733	1.658678
12	6	1.309131	-1.612960	1.859330
13	1	0.913006	-2.577041	1.504529
14	1	2.104454	-1.852325	2.593613
15	6	0.200210	-0.829234	2.557400
16	1	0.602606	0.128497	2.923226
17	1	-0.135114	-1.390372	3.453054
18	6	-1.785072	-1.664049	1.361156
19	1	-1.156356	-2.537417	1.126876
20	1	-2.435204	-1.944923	2.213153
21	6	-2.665353	-1.405760	0.121499
22	6	-1.681669	0.646800	2.118901
23	1	-2.704425	0.579281	1.716548
24	1	-1.774857	0.678389	3.220369
25	6	-1.132081	1.998251	1.618706
26	6	2.439254	-1.816184	-0.282313
27	1	3.044942	-1.222573	-0.985867
28	1	3.114551	-2.554358	0.191303
29	6	1.379586	-2.552355	-1.130033
30	6	2.732123	0.213210	1.024495
31	1	2.338424	0.740051	1.908343
32	1	3.755599	-0.121309	1.285349
33	6	2.815249	1.263652	-0.102156
34	8	-0.538152	1.075130	-2.486945
35	1	-1.520929	1.106190	-2.626657
36	1	-0.258945	2.010932	-2.289838
37	8	-3.262142	0.907322	-2.615233
38	1	-3.041943	0.269238	-1.869070
39	1	-3.562935	1.698335	-2.138788
40	8	0.504949	3.377811	-1.540615
41	1	1.267970	2.744457	-1.485930
42	1	0.061708	3.129466	-0.689395

E(UTPSSh) = -2479.3398008 Hartree
Zero-point correction = 0.311717
Thermal correction to Energy = 0.338784
Thermal correction to Enthalpy = 0.339728
Thermal correction to Gibbs Free Energy = 0.252819
Sum of electronic and zero-point Energies = -2479.028084
Sum of electronic and thermal Energies = -2479.001017
Sum of electronic and thermal Enthalpies = -2479.000073
Sum of electronic and thermal Free Energies = -2479.086982

$[Mn(EDTA)(H_2O)]^{2-}\cdot 3H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.033448	0.058049	0.339622

2	8	-2.262231	0.431963	0.130322
3	8	-3.789249	1.268146	-1.296702
4	8	-1.019773	-4.043990	-0.341890
5	8	-0.173067	-2.124819	0.469432
6	8	0.102862	2.197570	-0.058793
7	8	1.407824	3.935259	-0.637452
8	8	1.944674	-0.343477	1.407030
9	8	3.851392	-1.509551	1.142425
10	7	1.821039	0.384016	-1.178004
11	7	-0.831452	-0.730209	-1.804526
12	6	1.318421	0.278126	-2.554984
13	1	0.835582	1.235091	-2.806798
14	1	2.143466	0.142682	-3.282585
15	6	0.315290	-0.861616	-2.715398
16	1	0.807813	-1.820359	-2.489892
17	1	-0.008184	-0.917544	-3.774062
18	6	-1.799569	0.292749	-2.207510
19	1	-1.254953	1.198882	-2.516385
20	1	-2.423753	-0.022394	-3.066221
21	6	-2.720127	0.704475	-1.041577
22	6	-1.469898	-2.026428	-1.543392
23	1	-2.510915	-1.847379	-1.231548
24	1	-1.513579	-2.661513	-2.447498
25	6	-0.823750	-2.825044	-0.392340
26	6	2.307384	1.733700	-0.876337
27	1	2.949102	1.675389	0.017040
28	1	2.924758	2.152442	-1.693332
29	6	1.183548	2.725630	-0.519841
30	6	2.793757	-0.646987	-0.815878
31	1	2.464706	-1.612560	-1.231215
32	1	3.802217	-0.447661	-1.227977
33	6	2.899058	-0.849712	0.708811
34	8	-0.638367	0.245100	2.538269
35	1	-1.628226	0.209626	2.652278
36	1	-0.256447	-0.596380	2.920919
37	8	-3.330934	0.381491	2.504323
38	1	-3.098949	0.500852	1.532135
39	1	-3.699156	-0.516489	2.533204
40	8	0.675365	-2.019462	3.042372
41	1	1.390315	-1.443829	2.661598
42	1	0.297832	-2.349814	2.187853
43	8	-0.568318	3.063587	2.490242
44	1	-0.459275	2.960193	1.518298
45	1	-0.479365	2.128992	2.765420

E(UTPSSh) = -2555.7170704 Hartree
Zero-point correction = 0.336844
Thermal correction to Energy = 0.366361
Thermal correction to Enthalpy = 0.367306
Thermal correction to Gibbs Free Energy = 0.275183
Sum of electronic and zero-point Energies = -2555.380226
Sum of electronic and thermal Energies = -2555.350709
Sum of electronic and thermal Enthalpies = -2555.349765
Sum of electronic and thermal Free Energies = -2555.441887

$[Mn(EDTA)(H_2O)]^{2-}\cdot 4H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.086537	-0.087079	0.255764
2	8	1.931606	-1.345772	0.584299
3	8	3.413065	-2.653057	-0.494060
4	8	2.706942	3.261761	0.599288
5	8	0.978854	1.835980	0.794003
6	8	-0.761500	-1.942597	-0.529548

7	8	-2.276974	-2.915353	-1.876606
8	8	-1.842126	1.069709	0.830671
9	8	-2.925243	2.962480	0.275883
10	7	-1.166558	0.501790	-1.709914
11	7	1.753726	0.405858	-1.418789
12	6	-0.265444	0.454755	-2.871600
13	1	-0.147913	-0.602399	-3.156577
14	1	-0.703998	0.968927	-3.749713
15	6	1.101985	1.060094	-2.562823
16	1	0.986436	2.126277	-2.313025
17	1	1.734380	1.019364	-3.471827
18	6	2.330618	-0.905367	-1.727082
19	1	1.609723	-1.483250	-2.327104
20	1	3.264595	-0.834239	-2.317570
21	6	2.606418	-1.719631	-0.447603
22	6	2.720194	1.294165	-0.759831
23	1	3.439211	0.674285	-0.201339
24	1	3.305668	1.889032	-1.484915
25	6	2.090819	2.239118	0.283802
26	6	-2.211923	-0.523924	-1.793288
27	1	-2.982001	-0.302478	-1.036931
28	1	-2.698902	-0.554328	-2.785681
29	6	-1.711116	-1.924020	-1.407007
30	6	-1.718167	1.830504	-1.443947
31	1	-0.924363	2.583152	-1.571638
32	1	-2.532305	2.101691	-2.143911
33	6	-2.227427	1.983487	-0.000292
34	8	-0.122987	-0.573762	2.496392
35	1	0.735544	-0.920597	2.872259
36	1	-0.272254	0.339201	2.881906
37	8	2.232897	-1.686270	3.148475
38	1	2.268418	-1.709314	2.143219
39	1	2.861727	-0.982064	3.375953
40	8	-0.570662	2.002076	3.000039
41	1	-1.313895	1.812766	2.373354
42	1	0.137875	2.175694	2.327555
43	8	-1.754512	-2.716096	1.903446
44	1	-1.378391	-2.673244	0.990711
45	1	-1.257581	-1.977386	2.327245
46	8	-3.802040	-0.898061	1.317946
47	1	-3.186732	-0.138011	1.233423
48	1	-3.173132	-1.633053	1.517617

E(UTPSSh) = -2632.1023639 Hartree
Zero-point correction = 0.363080 (/Particle)
Thermal correction to Energy = 0.394597
Thermal correction to Enthalpy = 0.395541
Thermal correction to Gibbs Free Energy = 0.299293
Sum of electronic and zero-point Energies = -2631.739284
Sum of electronic and thermal Energies = -2631.707767
Sum of electronic and thermal Enthalpies = -2631.706823
Sum of electronic and thermal Free Energies = -2631.803070

$[Mn(EDTA)(H_2O)]^{2-}\cdot 5H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	-0.079899	0.004582	0.176390
2	8	1.603151	-0.906637	1.321134
3	8	2.426502	-2.861921	2.075191
4	8	3.612045	0.325392	-1.535205
5	8	1.417977	0.715318	-1.267226
6	8	-1.470251	-0.886015	1.581159

7	8	-3.559949	-1.635128	1.940386
8	8	-1.260813	1.742682	-0.739762
9	8	-2.137366	2.397267	-2.705751
10	7	-1.871601	-0.853617	-1.133609
11	7	0.843162	-1.969035	-1.013402
12	6	-1.579359	-2.247195	-1.508644
13	1	-1.753119	-2.869070	-0.616673
14	1	-2.278110	-2.613285	-2.286694
15	6	-0.144047	-2.435319	-1.997028
16	1	0.009607	-1.857816	-2.920146
17	1	0.005051	-3.501084	-2.262257
18	6	1.042573	-2.883740	0.114443
19	1	0.059923	-3.210404	0.492002
20	1	1.606126	-3.793681	-0.170009
21	6	1.769596	-2.184577	1.279777
22	6	2.128252	-1.549008	-1.600246
23	1	2.965821	-2.110862	-1.158059
24	1	2.149053	-1.770535	-2.681346
25	6	2.426439	-0.050066	-1.443893
26	6	-3.026051	-0.774463	-0.229835
27	1	-3.337532	0.280149	-0.149194
28	1	-3.887261	-1.366486	-0.590613
29	6	-2.679427	-1.168279	1.213925
30	6	-2.008226	0.052229	-2.276611
31	1	-1.229443	-0.182850	-3.019000
32	1	-2.982698	-0.057110	-2.790070
33	6	-1.806913	1.530207	-1.893845
34	8	0.489179	1.781889	1.540924
35	1	1.401252	1.617591	1.940394
36	1	0.651374	2.481841	0.851808
37	8	2.944945	1.183567	2.315032
38	1	2.651026	0.285122	2.007878
39	1	3.359085	1.601046	1.514200
40	8	0.964765	3.271835	-0.675300
41	1	-0.001652	3.112793	-0.802404
42	1	1.298319	2.395753	-1.013249
43	8	-1.606907	1.305427	3.247750
44	1	-1.615045	0.394420	2.869010
45	1	-0.836261	1.680212	2.759298
46	8	-3.208902	2.372787	1.213129
47	1	-2.521343	2.274618	0.519953
48	1	-2.748848	1.998952	2.003111
49	8	3.860443	2.481634	0.056507
50	1	3.797762	1.758043	-0.629915
51	1	3.097883	3.053163	-0.140690

E(UTPSSh) = -2708.4883145 Hartree
Zero-point correction = 0.389390
Thermal correction to Energy = 0.422738
Thermal correction to Enthalpy = 0.423683
Thermal correction to Gibbs Free Energy = 0.324470
Sum of electronic and zero-point Energies = -2708.098925
Sum of electronic and thermal Energies = -2708.065576
Sum of electronic and thermal Enthalpies = -2708.064632
Sum of electronic and thermal Free Energies = -2708.163845

[Mn(MeNO2A)(H_2O)], B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.039697	-0.531881	1.295011
2	6	-1.787490	0.694308	1.654830
3	6	-1.996569	1.673986	0.491019
4	6	0.260151	2.689345	0.580512
5	6	1.650952	2.051947	0.497934
6	7	1.626569	0.600230	0.758712
7	6	1.197478	0.240424	2.130155
8	6	0.095794	-0.829413	2.187360
9	1	-1.267343	1.201205	2.479102
10	1	-2.782054	0.432186	2.055299
11	1	-2.698589	1.240744	-0.235400
12	1	-2.468204	2.593786	0.890739
13	1	-0.080910	2.718681	1.624058
14	1	0.344311	3.745068	0.273027
15	1	2.050090	2.190373	-0.518232
16	1	2.328521	2.591080	1.189684
17	1	0.859282	1.147864	2.648561
18	1	2.056812	-0.127430	2.717165
19	1	0.508623	-1.797378	1.869885
20	1	-0.222341	-0.943617	3.242805
21	7	-0.754632	1.989169	-0.248750
22	6	-1.916434	-1.680767	1.030792
23	1	-1.320717	-2.604620	1.112594
24	1	-2.737066	-1.763693	1.765662
25	6	2.847484	-0.102246	0.341448
26	1	3.594803	-0.164510	1.152128
27	1	3.316477	0.463712	-0.480258
28	6	-2.517411	-1.692322	-0.396577
29	8	-1.836747	-1.064849	-1.291846
30	8	-3.550411	-2.329411	-0.589108
31	8	1.064201	0.497880	-2.652783
32	6	2.592499	-1.522662	-0.218592
33	8	1.447392	-1.697361	-0.781417
34	8	3.497693	-2.351135	-0.148169
35	25	-0.016515	-0.185299	-0.793537
36	1	1.650136	-0.235519	-2.899805
37	1	0.611131	0.752855	-3.471409
38	6	-1.051731	2.737774	-1.479752
39	1	-0.121793	2.924845	-2.034589
40	1	-1.725437	2.150593	-2.121239
41	1	-1.533905	3.710387	-1.264351

E(UB3LYP) = -2122.5287762 Hartree
Zero-point correction = 0.338768
Thermal correction to Energy = 0.360285
Thermal correction to Enthalpy = 0.361229
Thermal correction to Gibbs Free Energy = 0.287463
Sum of electronic and zero-point Energies = -2122.190008
Sum of electronic and thermal Energies = -2122.168491
Sum of electronic and thermal Enthalpies = -2122.167547
Sum of electronic and thermal Free Energies = -2122.241314

[Mn(MeNO2A)(H_2O)]·H_2O, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.597501	-0.275229	1.169014
2	6	-2.558511	0.803361	0.848831
3	6	-2.474047	1.313045	-0.596392
4	6	-0.513239	2.783862	-0.243217
5	6	0.887648	2.478533	0.297471
6	7	0.949596	1.208275	1.046340
7	6	0.120054	1.186176	2.271836
8	6	-0.804189	-0.035379	2.388853
9	1	-2.404987	1.637592	1.547105
10	1	-3.593073	0.461523	1.025910
11	1	-2.829937	0.532629	-1.284073
12	1	-3.158771	2.178120	-0.703312
13	1	-1.187107	3.047848	0.582766
14	1	-0.450059	3.691236	-0.867122
15	1	1.584739	2.386318	-0.548533
16	1	1.224122	3.340554	0.907570
17	1	-0.475991	2.108063	2.315439
18	1	0.761083	1.211021	3.170133
19	1	-0.193735	-0.933736	2.553444
20	1	-1.445673	0.097810	3.282891
21	7	-1.100998	1.662551	-1.019538
22	6	-2.194918	-1.615139	1.096483
23	1	-1.560629	-2.313494	1.666492
24	1	-3.201261	-1.653887	1.550723
25	6	2.316525	0.712109	1.250520
26	1	2.704866	0.946020	2.258416
27	1	2.994606	1.209811	0.540416
28	6	-2.270156	-2.193238	-0.338061
29	8	-1.395864	-1.740437	-1.167729
30	8	-3.102868	-3.066405	-0.572166
31	8	1.594916	-0.014176	-2.063368
32	6	2.498750	-0.796111	0.986001
33	8	1.484770	-1.446921	0.576319
34	8	3.649885	-1.252719	1.107603
35	25	0.036744	-0.360955	-0.539939
36	1	2.473995	-0.479795	-1.941677
37	1	1.392911	-0.065299	-3.008345
38	6	-1.049072	1.923739	-2.467069
39	1	-0.014366	2.136064	-2.770625
40	1	-1.395295	1.036507	-3.017820
41	8	3.945356	-1.215929	-1.624251
42	1	3.966659	-1.412757	-0.656325
43	1	4.652626	-0.564398	-1.744063
44	1	-1.683623	2.783918	-2.754446

E(UB3LYP) = -2198.9194377 Hartree
Zero-point correction = 0.364431
Thermal correction to Energy = 0.387841
Thermal correction to Enthalpy = 0.388786
Thermal correction to Gibbs Free Energy = 0.311090
Sum of electronic and zero-point Energies = -2198.555007
Sum of electronic and thermal Energies = -2198.531596
Sum of electronic and thermal Enthalpies = -2198.530652
Sum of electronic and thermal Free Energies = -2198.608348

[Mn(MeNO2A)(H_2O)]·$2H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.950036	-0.484662	0.819554
2	6	-2.706047	0.787508	0.848261

3	6	-2.285471	1.778160	-0.244272
4	6	-0.286350	2.618355	0.944381
5	6	0.941583	1.883995	1.490384
6	7	0.698364	0.434881	1.635985
7	6	-0.339297	0.101969	2.638669
8	6	-1.399027	-0.883204	2.128965
9	1	-2.582290	1.248728	1.838658
10	1	-3.787563	0.594910	0.740070
11	1	-2.582342	1.393575	-1.230769
12	1	-2.824464	2.733033	-0.084494
13	1	-1.079159	2.643699	1.704757
14	1	-0.014702	3.670797	0.758631
15	1	1.776594	2.003399	0.784121
16	1	1.245483	2.357048	2.444978
17	1	-0.822098	1.034416	2.965704
18	1	0.125725	-0.327722	3.543021
19	1	-0.937333	-1.869210	1.986884
20	1	-2.188301	-0.982986	2.900260
21	7	-0.821418	1.995395	-0.294220
22	6	-2.673389	-1.562785	0.130417
23	1	-2.226988	-2.523833	0.433601
24	1	-3.742533	-1.596027	0.408045
25	6	1.929336	-0.355529	1.779210
26	1	2.183092	-0.554148	2.836897
27	1	2.768576	0.217399	1.356068
28	6	-2.550453	-1.502003	-1.409391
29	8	-1.490771	-0.921499	-1.861574
30	8	-3.422690	-2.047946	-2.089372
31	8	1.793041	0.140745	-1.605097
32	6	1.915303	-1.683702	1.000651
33	8	0.899125	-1.932815	0.272676
34	8	2.945931	-2.386493	1.068466
35	25	-0.052124	-0.199113	-0.531385
36	1	2.436317	-0.625975	-1.622222
37	1	2.333985	0.971273	-1.592638
38	6	-0.454444	2.775178	-1.490823
39	1	0.634168	2.918764	-1.517074
40	1	-0.759063	2.223492	-2.392160
41	8	3.504634	-1.952952	-1.553788
42	8	3.158225	2.473797	-1.480005
43	1	3.383147	2.839365	-2.351701
44	1	4.012510	2.407889	-1.021888
45	1	3.346612	-2.309783	-0.638904
46	1	4.410733	-1.606473	-1.506978
47	1	-0.945810	3.766558	-1.496640

E(UB3LYP) = -2275.3016062 Hartree
Zero-point correction = 0.390762
Thermal correction to Energy = 0.416204
Thermal correction to Enthalpy = 0.417149
Thermal correction to Gibbs Free Energy = 0.336262
Sum of electronic and zero-point Energies = -2274.910844
Sum of electronic and thermal Energies = -2274.885402
Sum of electronic and thermal Enthalpies = -2274.884458
Sum of electronic and thermal Free Energies = -2274.965344

[Mn(MeNO2A)(H_2O)]·3H_2O, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.903642	-1.009079	-0.678477
2	6	-2.662401	-1.206822	0.578395
3	6	-2.246706	-0.266445	1.718804
4	6	-0.241048	-1.544304	2.404521
5	6	0.989723	-1.996582	1.608062

6	7	0.772258	-1.958686	0.147069
7	6	-0.272425	-2.889206	-0.331007
8	6	-1.328529	-2.245423	-1.241519
9	1	-2.558151	-2.252202	0.899588
10	1	-3.742204	-1.063537	0.400819
11	1	-2.552106	0.762248	1.480906
12	1	-2.795154	-0.563963	2.634706
13	1	-1.030186	-2.305755	2.343841
14	1	0.037556	-1.500224	3.470526
15	1	1.826169	-1.318978	1.833456
16	1	1.281182	-3.006760	1.959660
17	1	-0.762247	-3.349430	0.537782
18	1	0.182345	-3.727263	-0.887417
19	1	-0.860018	-1.973319	-2.197573
20	1	-2.107985	-3.002589	-1.459473
21	7	-0.787176	-0.234202	1.961158
22	6	-2.636453	-0.199513	-1.660697
23	1	-2.175086	-0.345249	-2.651177
24	1	-3.695663	-0.500098	-1.751449
25	6	2.016165	-1.990218	-0.639008
26	1	2.150192	-2.957027	-1.157325
27	1	2.883843	-1.882621	0.028599
28	6	-2.570196	1.318122	-1.379832
29	8	-1.502937	1.710366	-0.763874
30	8	-3.473308	2.042647	-1.783109
31	8	1.556920	1.818527	0.348400
32	6	2.133148	-0.863371	-1.686343
33	8	1.095532	-0.152660	-1.899044
34	8	3.241894	-0.684234	-2.218455
35	25	-0.020010	0.325054	-0.180011
36	1	2.183270	1.948906	-0.421982
37	1	2.136919	1.548124	1.103975
38	6	-0.438673	0.850877	2.899155
39	1	0.641284	0.825585	3.097603
40	1	-0.679329	1.825334	2.448575
41	8	3.300556	2.009026	-1.694327
42	8	3.080763	0.890999	2.397128
43	1	3.337038	1.521488	3.087501
44	1	3.917271	0.499975	2.102052
45	1	3.319439	1.087845	-2.059128
46	1	4.191766	2.139933	-1.338056
47	1	-0.977005	0.745606	3.860524
48	8	-0.539984	3.722603	0.912639
49	1	0.324908	3.283827	0.812513
50	1	-1.078993	3.186685	0.294930

E(UB3LYP) = -2351.6881441 Hartree
Zero-point correction = 0.416048
Thermal correction to Energy = 0.444463
Thermal correction to Enthalpy = 0.445407
Thermal correction to Gibbs Free Energy = 0.358032
Sum of electronic and zero-point Energies = -2351.272096
Sum of electronic and thermal Energies = -2351.243681
Sum of electronic and thermal Enthalpies = -2351.242737
Sum of electronic and thermal Free Energies = -2351.330112

[Mn(MeNO2A)(H_2O)]·4H_2O, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.683054	-1.961459	-0.905967
2	6	-0.871897	-2.882216	0.239429
3	6	-0.932825	-2.189443	1.609711
4	6	1.507482	-1.919227	1.891483

5	6	2.557723	-1.244506	1.003135
6	7	2.081504	-1.023573	-0.378179
7	6	1.804774	-2.274268	-1.122087
8	6	0.429436	-2.325884	-1.805475
9	1	-0.064009	-3.626367	0.233742
10	1	-1.802401	-3.462391	0.115579
11	1	-1.863641	-1.611805	1.693093
12	1	-0.964116	-2.971585	2.393937
13	1	1.389322	-2.971743	1.602353
14	1	1.892825	-1.942477	2.924341
15	1	2.801613	-0.258762	1.427003
16	1	3.485063	-1.850535	1.032017
17	1	1.908404	-3.124665	-0.434065
18	1	2.570239	-2.434628	-1.900920
19	1	0.415268	-1.607306	-2.636124
20	1	0.297730	-3.337402	-2.238616
21	7	0.182724	-1.246313	1.848876
22	6	-1.935641	-1.650104	-1.606561
23	1	-1.696234	-1.266678	-2.611514
24	1	-2.576242	-2.538561	-1.751340
25	6	2.880834	-0.039350	-1.127114
26	1	3.559349	-0.521851	-1.853794
27	1	3.526639	0.516283	-0.431143
28	6	-2.761501	-0.543345	-0.921310
29	8	-2.106276	0.218105	-0.119790
30	8	-3.954762	-0.417401	-1.205274
31	8	0.239689	2.167470	0.817651
32	6	2.041170	1.021729	-1.867366
33	8	0.773790	0.879503	-1.846281
34	8	2.644299	1.979271	-2.379511
35	25	0.009286	0.130014	-0.030020
36	1	0.495466	2.815782	0.098355
37	1	0.963287	2.233578	1.491010
38	6	-0.057288	-0.443099	3.063274
39	1	0.798170	0.224250	3.234371
40	1	-0.952918	0.181921	2.929963
41	8	1.066001	3.850165	-1.120274
42	8	2.290904	2.147142	2.586887
43	1	2.185377	2.645384	3.411825
44	1	3.123239	2.472514	2.211321
45	1	1.595269	3.278535	-1.731322
46	1	1.716235	4.466419	-0.751939
47	1	-0.193712	-1.083448	3.955300
48	8	-2.507694	2.100195	1.792947
49	1	-1.613084	2.420403	1.567333
50	1	-2.557552	1.315594	1.204973
51	8	-4.612677	2.272781	-0.314265
52	1	-3.931914	2.419660	0.365251
53	1	-4.447837	1.349382	-0.593019

E(UB3LYP) = -2428.0709577 Hartree
Zero-point correction = 0.440721
Thermal correction to Energy = 0.472087
Thermal correction to Enthalpy = 0.473031
Thermal correction to Gibbs Free Energy = 0.378081
Sum of electronic and zero-point Energies = -2427.630237
Sum of electronic and thermal Energies = -2427.598870
Sum of electronic and thermal Enthalpies = -2427.597926
Sum of electronic and thermal Free Energies = -2427.692877

[Mn(MeNO2A)(H_2O)], TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.030333	-0.565348	1.264132

2	6	-1.792433	0.643180	1.656700
3	6	-2.021866	1.629447	0.505111
4	6	0.220215	2.668792	0.620541
5	6	1.617716	2.051896	0.522197
6	7	1.597288	0.593790	0.758403
7	6	1.179832	0.212956	2.128757
8	6	0.099826	-0.877165	2.160401
9	1	-1.260355	1.144375	2.477857
10	1	-2.776611	0.357931	2.066651
11	1	-2.712519	1.192180	-0.229771
12	1	-2.501614	2.541446	0.911726
13	1	-0.126003	2.661600	1.663530
14	1	0.281769	3.731479	0.333076
15	1	2.009307	2.201909	-0.495116
16	1	2.293857	2.580733	1.222198
17	1	0.818780	1.110508	2.650379
18	1	2.048711	-0.142559	2.708950
19	1	0.525485	-1.830424	1.815423
20	1	-0.225922	-1.020767	3.209301
21	7	-0.777189	1.961290	-0.225656
22	6	-1.900425	-1.715296	0.973652
23	1	-1.287623	-2.630808	1.012667
24	1	-2.708086	-1.829615	1.718664
25	6	2.830400	-0.088844	0.335840
26	1	3.578850	-0.138651	1.146294
27	1	3.279415	0.489233	-0.488370
28	6	-2.516605	-1.669088	-0.444345
29	8	-1.841932	-1.003315	-1.321622
30	8	-3.555441	-2.297166	-0.655552
31	8	1.239917	0.589031	-2.552960
32	6	2.584071	-1.509154	-0.221802
33	8	1.442337	-1.683536	-0.800388
34	8	3.488373	-2.342473	-0.140496
35	25	-0.015497	-0.169284	-0.790429
36	1	1.761481	-0.203646	-2.771989
37	1	0.827178	0.856667	-3.391651
38	6	-1.081310	2.720221	-1.452107
39	1	-0.147534	2.941566	-1.987028
40	1	-1.727086	2.115195	-2.105333
41	1	-1.594976	3.673617	-1.226424

E(UTPSSh) = -2122.5764494 Hartree
Zero-point correction = 0.338060
Thermal correction to Energy = 0.359576
Thermal correction to Enthalpy = 0.360520
Thermal correction to Gibbs Free Energy = 0.287693
Sum of electronic and zero-point Energies = -2122.238389
Sum of electronic and thermal Energies = -2122.216874
Sum of electronic and thermal Enthalpies = -2122.215929
Sum of electronic and thermal Free Energies = -2122.288756

[Mn(MeNO2A)(H_2O)]·H_2O, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.550687	-0.244320	-1.190546
2	6	2.578072	0.752214	-0.809753
3	6	2.532936	1.143777	0.672082
4	6	0.659971	2.744434	0.441026
5	6	-0.761895	2.557898	-0.093297
6	7	-0.887559	1.346561	-0.929911
7	6	-0.075191	1.383824	-2.167658
8	6	0.771323	0.123326	-2.388606
9	1	2.452426	1.645770	-1.437876
10	1	3.587809	0.366849	-1.033602

11	1	2.839923	0.289261	1.291788
12	1	3.260114	1.961114	0.846610
13	1	1.340718	3.014650	-0.378285
14	1	0.667418	3.603817	1.132031
15	1	-1.452893	2.429707	0.753410
16	1	-1.063462	3.475057	-0.636417
17	1	0.574055	2.270382	-2.135650
18	1	-0.725420	1.520993	-3.048917
19	1	0.107951	-0.725632	-2.605440
20	1	1.417856	0.282560	-3.273981
21	7	1.176371	1.528874	1.121989
22	6	2.075765	-1.617713	-1.223686
23	1	1.384715	-2.236258	-1.819385
24	1	3.067260	-1.676637	-1.707597
25	6	-2.283463	0.944002	-1.156635
26	1	-2.662824	1.279987	-2.138711
27	1	-2.920180	1.420249	-0.395651
28	6	2.150080	-2.281062	0.171108
29	8	1.319590	-1.826707	1.049180
30	8	2.937931	-3.214398	0.336193
31	8	-1.655830	-0.066684	2.000155
32	6	-2.533452	-0.566881	-1.007202
33	8	-1.545311	-1.299420	-0.667810
34	8	-3.710074	-0.962566	-1.139915
35	25	-0.053217	-0.362500	0.505272
36	1	-2.476781	-0.636620	1.856053
37	1	-1.462472	-0.124819	2.949115
38	6	1.132524	1.675470	2.587301
39	1	0.110593	1.930641	2.900655
40	1	1.418533	0.724003	3.059325
41	8	-3.824334	-1.535846	1.518002
42	1	-3.882806	-1.521157	0.525304
43	1	-4.603234	-1.027706	1.798892
44	1	1.818835	2.467721	2.941304

E(UTPSSh) = -2198.9615587 Hartree
Zero-point correction = 0.363721
Thermal correction to Energy = 0.387050
Thermal correction to Enthalpy = 0.387995
Thermal correction to Gibbs Free Energy = 0.311158
Sum of electronic and zero-point Energies = -2198.597838
Sum of electronic and thermal Energies = -2198.574508
Sum of electronic and thermal Enthalpies = -2198.573564
Sum of electronic and thermal Free Energies = -2198.650401

[Mn(MeNO2A)(H_2O)]·2H_2O, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.950036	-0.484662	0.819554
2	6	-2.706047	0.787508	0.848261
3	6	-2.285471	1.778160	-0.244272
4	6	-0.286350	2.618355	0.944381
5	6	0.941583	1.883995	1.490384
6	7	0.698364	0.434881	1.635985
7	6	-0.339297	0.101969	2.638669
8	6	-1.399027	-0.883204	2.128965
9	1	-2.582290	1.248728	1.838658
10	1	-3.787563	0.594910	0.740070
11	1	-2.582342	1.393575	-1.230769
12	1	-2.824464	2.733033	-0.084494

13	1	-1.079159	2.643699	1.704757
14	1	-0.014702	3.670797	0.758631
15	1	1.776594	2.003399	0.784121
16	1	1.245483	2.357048	2.444978
17	1	-0.822098	1.034416	2.965704
18	1	0.125725	-0.327722	3.543021
19	1	-0.937333	-1.869210	1.986884
20	1	-2.188301	-0.982986	2.900260
21	7	-0.821418	1.995395	-0.294220
22	6	-2.673389	-1.562785	0.130417
23	1	-2.226988	-2.523833	0.433601
24	1	-3.742533	-1.596027	0.408045
25	6	1.929336	-0.355529	1.779210
26	1	2.183092	-0.554148	2.836897
27	1	2.768576	0.217399	1.356068
28	6	-2.550453	-1.502003	-1.409391
29	8	-1.490771	-0.921499	-1.861574
30	8	-3.422690	-2.047946	-2.089372
31	8	1.793041	0.140745	-1.605097
32	6	1.915303	-1.683702	1.000651
33	8	0.899125	-1.932815	0.272676
34	8	2.945931	-2.386493	1.068466
35	25	-0.052124	-0.199113	-0.531385
36	1	2.436317	-0.625975	-1.622222
37	1	2.333985	0.971273	-1.592638
38	6	-0.454444	2.775178	-1.490823
39	1	0.634168	2.918764	-1.517074
40	1	-0.759063	2.223492	-2.392160
41	8	3.504634	-1.952952	-1.553788
42	8	3.158225	2.473797	-1.480005
43	1	3.383147	2.839365	-2.351701
44	1	4.012510	2.407889	-1.021888
45	1	3.346612	-2.309783	-0.638904
46	1	4.410733	-1.606473	-1.506978
47	1	-0.945810	3.766558	-1.496640

E(UTPSSh) = -2275.3385157 Hartree
Zero-point correction = 0.388757
Thermal correction to Energy = 0.415052
Thermal correction to Enthalpy = 0.415996
Thermal correction to Gibbs Free Energy = 0.332588
Sum of electronic and zero-point Energies = -2274.949758
Sum of electronic and thermal Energies = -2274.923464
Sum of electronic and thermal Enthalpies = -2274.922520
Sum of electronic and thermal Free Energies = -2275.005928

[Mn(MeNO2A)(H_2O)]·3H_2O, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.878419	-0.963542	-0.732696
2	6	-2.675307	-1.205172	0.493769
3	6	-2.286606	-0.294216	1.665050
4	6	-0.322491	-1.623132	2.363573
5	6	0.928548	-2.057671	1.592796
6	7	0.744506	-1.949493	0.129142
7	6	-0.287302	-2.866341	-0.406534
8	6	-1.305000	-2.185647	-1.330999
9	1	-2.563941	-2.259180	0.785318
10	1	-3.749746	-1.062479	0.286593
11	1	-2.566421	0.744646	1.439823
12	1	-2.856095	-0.605797	2.562533
13	1	-1.121728	-2.367597	2.240825

14	1	-0.086538	-1.612146	3.440484
15	1	1.765615	-1.396552	1.862998
16	1	1.201050	-3.085037	1.904767
17	1	-0.808172	-3.336255	0.439776
18	1	0.185274	-3.692579	-0.965280
19	1	-0.802831	-1.876440	-2.258418
20	1	-2.087047	-2.923287	-1.597983
21	7	-0.829571	-0.292838	1.933217
22	6	-2.582566	-0.111150	-1.702090
23	1	-2.081987	-0.213124	-2.678857
24	1	-3.636904	-0.411525	-1.839005
25	6	2.012001	-1.970471	-0.622361
26	1	2.179581	-2.943126	-1.119484
27	1	2.851126	-1.828660	0.074853
28	6	-2.525513	1.387531	-1.339067
29	8	-1.479261	1.740793	-0.659828
30	8	-3.411575	2.140332	-1.738415
31	8	1.578613	1.760961	0.385158
32	6	2.125346	-0.849187	-1.671859
33	8	1.087047	-0.133886	-1.881754
34	8	3.236562	-0.669169	-2.208148
35	25	-0.016262	0.309657	-0.144885
36	1	2.193416	1.905103	-0.400753
37	1	2.174015	1.479150	1.131749
38	6	-0.477745	0.767753	2.899497
39	1	0.597242	0.711842	3.118456
40	1	-0.688127	1.752284	2.454861
41	8	3.247748	2.009101	-1.692510
42	8	3.109289	0.867551	2.421166
43	1	3.358664	1.543243	3.073439
44	1	3.957051	0.493960	2.127943
45	1	3.276123	1.081650	-2.055909
46	1	4.148147	2.155260	-1.359271
47	1	-1.040971	0.657343	3.845268
48	8	-0.450280	3.710194	0.987216
49	1	0.401119	3.240316	0.874378
50	1	-1.012309	3.187873	0.371648

E(UTPSSh) = -2351.7181958 Hartree
Zero-point correction = 0.413987
Thermal correction to Energy = 0.442815
Thermal correction to Enthalpy = 0.443759
Thermal correction to Gibbs Free Energy = 0.354883
Sum of electronic and zero-point Energies = -2351.304209
Sum of electronic and thermal Energies = -2351.275381
Sum of electronic and thermal Enthalpies = -2351.274437
Sum of electronic and thermal Free Energies = -2351.363312

[Mn(MeNO2A)(H_2O)]·4H_2O, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.363506	-1.964872	-1.030366
2	6	-0.291514	-3.044694	-0.016576
3	6	-0.381590	-2.551691	1.434957
4	6	1.974389	-1.831065	1.617136
5	6	2.802085	-0.849199	0.783393
6	7	2.179761	-0.583066	-0.531011
7	6	2.104901	-1.776470	-1.406535

8	6	0.722572	-2.007235	-2.030945
9	1	0.646177	-3.598999	-0.165370
10	1	-1.100925	-3.776900	-0.178989
11	1	-1.395885	-2.184963	1.642085
12	1	-0.189124	-3.408296	2.110099
13	1	2.028867	-2.837256	1.178964
14	1	2.424898	-1.913526	2.619979
15	1	2.863652	0.113535	1.313185
16	1	3.832749	-1.242986	0.686706
17	1	2.401261	-2.657554	-0.819853
18	1	2.841827	-1.697452	-2.224188
19	1	0.514376	-1.207894	-2.754937
20	1	0.742600	-2.968730	-2.580529
21	7	0.545415	-1.431430	1.722698
22	6	-1.699847	-1.813778	-1.624638
23	1	-1.599639	-1.277270	-2.581539
24	1	-2.176298	-2.785124	-1.850650
25	6	2.713862	0.613509	-1.203237
26	1	3.452609	0.356893	-1.983873
27	1	3.242676	1.234932	-0.464804
28	6	-2.655542	-0.970908	-0.761436
29	8	-2.102763	-0.313886	0.198460
30	8	-3.855217	-0.929097	-1.059383
31	8	-0.190352	2.104030	0.975569
32	6	1.621769	1.509973	-1.815028
33	8	0.413191	1.105725	-1.721414
34	8	1.974856	2.603179	-2.299201
35	25	-0.015339	0.074359	0.072809
36	1	-0.109921	2.824950	0.274344
37	1	0.551474	2.277147	1.616630
38	6	0.248015	-0.821120	3.035350
39	1	0.952861	0.001360	3.218572
40	1	-0.771152	-0.406870	3.025622
41	8	0.120076	4.005229	-0.879597
42	8	1.919329	2.351638	2.639924
43	1	1.763184	2.774797	3.500754
44	1	2.652151	2.859613	2.253647
45	1	0.726242	3.581534	-1.547350
46	1	0.657764	4.719656	-0.500526
47	1	0.331475	-1.558499	3.855273
48	8	-2.784620	1.571292	2.018960
49	1	-1.926070	1.983470	1.777776
50	1	-2.725642	0.748021	1.478787
51	8	-4.428409	1.819085	-0.354442
52	1	-3.918676	1.900005	0.478905
53	1	-4.345067	0.861512	-0.553846

E(UTPSSh) = -2428.0962599 Hartree
Zero-point correction = 0.439532
Thermal correction to Energy = 0.469718
Thermal correction to Enthalpy = 0.470663
Thermal correction to Gibbs Free Energy = 0.379827
Sum of electronic and zero-point Energies = -2427.656728
Sum of electronic and thermal Energies = -2427.626541
Sum of electronic and thermal Enthalpies = -2427.625597
Sum of electronic and thermal Free Energies = -2427.716433

[Mn(MeNO2A)(H_2O)]·5H_2O, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.316904	-2.157017	-0.751013
2	6	0.332500	-3.013746	0.460665
3	6	-0.066101	-2.274342	1.744418
4	6	2.146292	-1.233253	2.125859
5	6	2.994688	-0.316239	1.240834
6	7	2.579190	-0.377090	-0.177583
7	6	2.778785	-1.708136	-0.797984
8	6	1.553679	-2.229980	-1.557562
9	1	1.336680	-3.446639	0.572433
10	1	-0.350636	-3.870089	0.330834
11	1	-1.131065	-2.003616	1.706555
12	1	0.071733	-2.959165	2.603773
13	1	2.380333	-2.286443	1.917318
14	1	2.428598	-1.067091	3.178404
15	1	2.865268	0.725441	1.571291
16	1	4.062231	-0.579304	1.373636
17	1	3.062167	-2.421423	-0.011006
18	1	3.630255	-1.680542	-1.499330
19	1	1.386102	-1.607549	-2.447444
20	1	1.763822	-3.262243	-1.898830
21	7	0.686415	-1.013653	1.942859
22	6	-0.905711	-2.328403	-1.548036
23	1	-0.719075	-1.944214	-2.564064
24	1	-1.200906	-3.387698	-1.649689
25	6	3.097654	0.742214	-0.986626
26	1	3.931411	0.425594	-1.638634
27	1	3.500871	1.518431	-0.319695
28	6	-2.094122	-1.521930	-1.000800
29	8	-1.794183	-0.495256	-0.290082
30	8	-3.240608	-1.875263	-1.315764
31	8	-0.268892	2.168411	0.524663
32	6	2.019630	1.422447	-1.850321
33	8	0.870295	0.864216	-1.894788
34	8	2.312011	2.499945	-2.404279
35	25	0.252402	0.070664	-0.050233
36	1	-0.206103	2.778735	-0.277029
37	1	0.386315	2.535940	1.178355
38	6	0.114214	-0.231276	3.058851
39	1	0.712444	0.678816	3.202322
40	1	-0.914200	0.069195	2.809517
41	8	0.041851	3.769060	-1.588983
42	8	1.621011	2.982208	2.274104
43	1	1.322742	3.513006	3.031580
44	1	2.312659	3.524420	1.859521
45	1	0.825323	3.360512	-2.050747
46	1	0.373904	4.628511	-1.281975
47	1	0.113743	-0.812189	4.000010
48	8	-2.717650	1.249404	1.599310
49	1	-1.974909	1.829479	1.322458
50	1	-2.627620	0.525662	0.935383
51	8	-5.276674	-0.092291	-1.157154
52	1	-4.963931	0.568423	-1.795393
53	1	-4.530823	-0.752011	-1.137954
54	8	-5.438403	1.672614	1.028494

55	1	-5.441795	1.007636	0.303639
56	1	-4.492273	1.669609	1.290805

E(UTPSSh) = -2504.4744574 Hartree
Zero-point correction = 0.463674
Thermal correction to Energy = 0.497902
Thermal correction to Enthalpy = 0.498846
Thermal correction to Gibbs Free Energy = 0.396626
Sum of electronic and zero-point Energies = -2504.010783
Sum of electronic and thermal Energies = -2503.976556
Sum of electronic and thermal Enthalpies = -2503.975612
Sum of electronic and thermal Free Energies = -2504.077832

$[Mn(CyDTA)(H_2O)]^{2-}\cdot 4H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.832951	0.212806	0.028786
2	8	1.094278	2.130892	-1.097565
3	8	0.168017	3.387075	-2.708480
4	8	-0.471471	2.661373	3.260934
5	8	0.543786	1.110336	1.999875
6	8	0.890425	-0.730846	-1.926474
7	8	0.310915	-2.460590	-3.228686
8	8	1.457088	-1.591594	1.308289
9	8	0.647331	-2.838355	2.987547
10	7	-0.945231	-1.495945	0.018023
11	7	-1.310522	1.431306	-0.054051
12	6	-2.239135	-0.890777	-0.391015
13	1	-2.173220	-0.763472	-1.485092
14	6	-2.447247	0.515048	0.221491
15	1	-2.464557	0.389771	1.317440
16	6	-1.277956	2.005364	-1.403241
17	1	-1.502117	1.217554	-2.139856
18	1	-2.020610	2.809004	-1.559067
19	6	0.104317	2.576494	-1.783323
20	6	-1.172834	2.454810	0.990833
21	1	-0.663516	3.333733	0.566424
22	1	-2.147010	2.818210	1.362876
23	6	-0.316735	2.040918	2.207622
24	6	-0.455798	-2.465673	-0.968154
25	1	0.317115	-3.092697	-0.498650
26	1	-1.246209	-3.140353	-1.341912
27	6	0.280370	-1.840500	-2.165242
28	6	-0.909971	-2.025302	1.382638
29	1	-1.421134	-1.323291	2.059653
30	1	-1.423537	-2.998598	1.489776
31	6	0.512276	-2.187883	1.951552
32	8	3.139928	0.514917	0.224555
33	1	3.403973	1.439281	-0.022436
34	1	3.264329	0.421988	1.206180
35	8	3.538096	3.011821	-0.731985
36	1	2.603782	2.822456	-1.031744
37	1	3.417532	3.650673	-0.013959
38	8	2.918077	0.077876	2.867429
39	1	2.565337	-0.769440	2.510594
40	1	2.091427	0.613605	2.818874
41	6	-3.454511	-1.802255	-0.105156
42	1	-3.508714	-2.002655	0.978045
43	1	-3.300999	-2.777193	-0.595249
44	6	-3.814617	1.103023	-0.193480
45	1	-3.811647	1.296008	-1.279319

46	1	-3.954031	2.080108	0.296961
47	6	-4.784963	-1.185765	-0.545680
48	1	-5.613198	-1.871462	-0.301506
49	1	-4.795057	-1.059175	-1.643607
50	6	-4.987906	0.173500	0.125461
51	1	-5.932545	0.636429	-0.204797
52	1	-5.071143	0.034966	1.218830
53	8	3.610709	-1.066728	-2.009685
54	1	2.663252	-0.920671	-2.231830
55	1	3.674054	-0.548944	-1.178962
56	8	2.916104	-3.286818	-0.432060
57	1	3.208771	-2.605217	-1.075960
58	1	2.488159	-2.739172	0.255427

E(UB3LYP) = -2788.0342723 Hartree
Zero-point correction = 0.458794
Thermal correction to Energy = 0.493649
Thermal correction to Enthalpy = 0.494593
Thermal correction to Gibbs Free Energy = 0.392007
Sum of electronic and zero-point Energies = -2787.575478
Sum of electronic and thermal Energies = -2787.540623
Sum of electronic and thermal Enthalpies = -2787.539679
Sum of electronic and thermal Free Energies = -2787.642265

$[Mn(CyDTA)(H_2O)]^{2-}\cdot 4H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.808724	0.196984	0.025380
2	8	1.111521	2.124526	-1.074646
3	8	0.202376	3.365645	-2.715823
4	8	-0.434414	2.655226	3.262895
5	8	0.528661	1.053638	2.012953
6	8	0.836300	-0.694606	-1.954238
7	8	0.237899	-2.422025	-3.261805
8	8	1.461974	-1.609949	1.277955
9	8	0.663508	-2.873972	2.957365
10	7	-0.931376	-1.480701	0.017194
11	7	-1.271150	1.424017	-0.050793
12	6	-2.226259	-0.873014	-0.388150
13	1	-2.159440	-0.738744	-1.482099
14	6	-2.417051	0.523447	0.240285
15	1	-2.415534	0.393124	1.336670
16	6	-1.254495	1.994906	-1.403910
17	1	-1.483293	1.200397	-2.132281
18	1	-1.999497	2.798073	-1.551693
19	6	0.127858	2.562786	-1.780754
20	6	-1.124655	2.457695	0.985252
21	1	-0.581445	3.311990	0.552065
22	1	-2.096941	2.847925	1.335635
23	6	-0.297412	2.022031	2.211070
24	6	-0.453092	-2.455360	-0.972442
25	1	0.347054	-3.055751	-0.510959
26	1	-1.244080	-3.146606	-1.314370
27	6	0.232523	-1.813121	-2.187799
28	6	-0.906152	-2.022175	1.379283
29	1	-1.404378	-1.310852	2.057218
30	1	-1.435687	-2.987793	1.476342
31	6	0.518033	-2.207620	1.929340
32	8	3.104053	0.506813	0.226431
33	1	3.367023	1.442217	-0.001092
34	1	3.222359	0.396284	1.213882
35	8	3.528309	3.010156	-0.673505
36	1	2.590897	2.819497	-0.984621
37	1	3.395140	3.634626	0.058183

38	8	2.895823	0.038611	2.846237
39	1	2.547393	-0.810633	2.476045
40	1	2.056953	0.565974	2.802382
41	6	-3.441607	-1.779984	-0.098222
42	1	-3.485447	-1.984851	0.985077
43	1	-3.297508	-2.751490	-0.598519
44	6	-3.779825	1.128969	-0.157500
45	1	-3.782052	1.327155	-1.242860
46	1	-3.904419	2.103186	0.342962
47	6	-4.770380	-1.147809	-0.523139
48	1	-5.601588	-1.829543	-0.279233
49	1	-4.785363	-1.007241	-1.619020
50	6	-4.956225	0.204815	0.167089
51	1	-5.900719	0.678055	-0.147645
52	1	-5.024460	0.054002	1.259598
53	8	3.550949	-1.037960	-2.013080
54	1	2.599903	-0.888507	-2.236035
55	1	3.610013	-0.524511	-1.173267
56	8	2.922994	-3.280300	-0.460657
57	1	3.190483	-2.578638	-1.101759
58	1	2.487034	-2.744995	0.237005

E(UTPSSh) = -2788.0591319 Hartree
Zero-point correction = 0.456096
Thermal correction to Energy = 0.491152
Thermal correction to Enthalpy = 0.492097
Thermal correction to Gibbs Free Energy = 0.388752
Sum of electronic and zero-point Energies = -2787.603036
Sum of electronic and thermal Energies = -2787.567979
Sum of electronic and thermal Enthalpies = -2787.567035
Sum of electronic and thermal Free Energies = -2787.670380

[Mn(L1)(H_2O)]·4H_2O, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.148884	0.272172	-0.292516
2	15	-2.672494	-0.515455	0.921261
3	8	-0.120182	2.271828	-1.430479
4	8	-1.807753	0.695086	0.290313
5	8	-3.855566	0.013773	1.726473
6	8	-3.031005	-1.543372	-0.186264
7	7	2.318694	-0.173302	-0.425403
8	7	0.292240	-1.762587	-1.330402
9	7	-0.004529	-1.225453	1.576267
10	7	1.170885	1.518085	1.391361
11	6	2.708900	-1.249209	-1.128483
12	6	4.040869	-1.674180	-1.106594
13	1	4.350187	-2.552075	-1.676586
14	6	4.956194	-0.959333	-0.327278
15	1	6.001375	-1.273405	-0.285457
16	6	4.526289	0.144241	0.416565
17	1	5.218842	0.702737	1.048695
18	6	3.179424	0.513517	0.344196
19	6	1.616980	-1.926373	-1.940253
20	1	1.592277	-1.452085	-2.935934
21	1	1.874037	-2.988813	-2.097180
22	6	-0.107116	-2.800675	-0.357491
23	1	0.227117	-3.802797	-0.684469
24	1	-1.206841	-2.793433	-0.324841
25	6	0.436682	-2.533751	1.045564
26	1	0.127988	-3.358720	1.716375
27	1	1.536742	-2.531691	1.027922
28	6	0.937757	-0.679683	2.579480

29	1	1.952798	-0.987967	2.288309
30	1	0.750278	-1.107396	3.582761
31	6	0.874753	0.845472	2.672449
32	1	-0.138057	1.160362	2.966061
33	1	1.563681	1.179183	3.470003
34	6	2.591329	1.714469	1.058799
35	1	2.641549	2.558946	0.347667
36	1	3.200239	1.969755	1.943572
37	6	-1.407814	-1.240411	2.077056
38	1	-1.467212	-0.613652	2.980052
39	1	-1.701942	-2.261998	2.378650
40	1	0.694348	2.424338	1.394755
41	1	-0.449051	-1.685972	-2.052714
42	1	-0.869204	2.184549	-2.057999
43	1	-0.515968	2.805239	-0.674955
44	8	-2.749050	1.380254	-2.118001
45	8	-1.187370	3.175226	0.809976
46	1	-1.644126	2.282446	0.792643
47	1	-1.889580	3.844043	0.833520
48	1	-2.403001	1.141575	-1.213144
49	1	-3.709448	1.227847	-1.952203
50	8	-2.161976	-1.301934	-2.721013
51	1	-2.291454	-0.324294	-2.742866
52	1	-2.514076	-1.493485	-1.807920
53	8	2.305765	3.696267	-1.657270
54	1	1.450190	3.219300	-1.729094
55	1	2.053537	4.524592	-1.219293
56	8	-5.044050	0.304115	-0.894750
57	1	-4.527211	-0.535024	-0.918519
58	1	-4.899712	0.513755	0.057462

E(UTPSSh) = -2863.43839923 Hartree
Zero-point correction = 0.476270
Thermal correction to Energy = 0.509765
Thermal correction to Enthalpy = 0.510709
Thermal correction to Gibbs Free Energy = 0.412662
Sum of electronic and zero-point Energies = -2862.962130
Sum of electronic and thermal Energies = -2862.928635
Sum of electronic and thermal Enthalpies = -2862.927691
Sum of electronic and thermal Free Energies = -2863.025738

$[Mn(L2)(H_2O)]^+ \cdot 4H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.393395	0.274118	0.204806
2	8	0.885466	1.952243	1.568867
3	7	-1.776286	-0.318488	0.361880
4	7	0.351961	-1.967853	0.901392
5	7	0.469196	-0.849772	-1.898451
6	7	-0.807497	1.743994	-1.191027
7	6	-2.098830	-1.518612	0.861400
8	6	-3.421240	-1.973086	0.841109
9	1	-3.673643	-2.955558	1.244729
10	6	-4.400773	-1.148541	0.282999
11	1	-5.441507	-1.479148	0.249119
12	6	-4.041336	0.091475	-0.252757
13	1	-4.785026	0.743216	-0.715095
14	6	-2.699788	0.478378	-0.197400
15	6	-0.957033	-2.319280	1.463879
16	1	-0.928188	-2.099513	2.544835
17	1	-1.174851	-3.398534	1.371357
18	6	0.783563	-2.749681	-0.270530

19	1	0.528625	-3.819745	-0.153479
20	1	1.880726	-2.694755	-0.321558
21	6	0.165290	-2.262322	-1.585640
22	1	0.506111	-2.928478	-2.401519
23	1	-0.927548	-2.371105	-1.531424
24	6	-0.551358	-0.212856	-2.757908
25	1	-1.527382	-0.647063	-2.499939
26	1	-0.383025	-0.442091	-3.827579
27	6	-0.609391	1.310281	-2.585961
28	1	0.333713	1.761043	-2.931850
29	1	-1.403902	1.701593	-3.248297
30	6	-2.191969	1.814267	-0.704284
31	1	-2.191319	2.499327	0.162175
32	1	-2.885374	2.220933	-1.461768
33	6	1.843533	-0.670938	-2.397924
34	1	1.878106	0.213551	-3.053498
35	1	2.165838	-1.526712	-3.017439
36	1	-0.361061	2.655307	-1.058144
37	1	1.058455	-2.031027	1.641461
38	1	1.748626	1.650272	1.993716
39	1	1.091874	2.737628	1.006145
40	8	3.140985	0.823750	2.294867
41	8	1.001395	3.974319	-0.242699
42	1	1.803002	4.146748	-0.760695
43	1	0.699166	4.849539	0.045810
44	1	2.886533	-0.008382	2.747932
45	1	3.192026	0.539348	1.350512
46	6	2.915423	-0.416762	-1.315748
47	8	2.478098	0.088794	-0.211135
48	8	4.089272	-0.653442	-1.581334
49	8	2.261602	-1.691010	3.214285
50	1	1.797758	-1.740907	4.064759
51	1	2.967225	-2.352823	3.286235
52	8	-1.596947	3.032199	2.413801
53	1	-2.133527	2.286295	2.716969
54	1	-0.713438	2.634164	2.279208

E(UB3LYP) = -2408.4715925 Hartree
Zero-point correction = 0.451284 (Hartree/Particle)
Thermal correction to Energy = 0.482810
Thermal correction to Enthalpy = 0.483754
Thermal correction to Gibbs Free Energy = 0.387782
Sum of electronic and zero-point Energies = -2408.020309
Sum of electronic and thermal Energies = -2407.988782
Sum of electronic and thermal Enthalpies = -2407.987838
Sum of electronic and thermal Free Energies = -2408.083810

$[Mn(L2)(H_2O)]^{+}\cdot 4H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	25	0.390801	0.264740	0.198222
2	8	0.933392	1.931325	1.538113
3	7	-1.769002	-0.296411	0.368911
4	7	0.334801	-1.952618	0.901626
5	7	0.422461	-0.836555	-1.880416
6	7	-0.783959	1.759336	-1.158519
7	6	-2.107154	-1.497582	0.862679
8	6	-3.434158	-1.939996	0.836515
9	1	-3.696176	-2.922121	1.234073
10	6	-4.405721	-1.102264	0.282011
11	1	-5.448730	-1.423601	0.242825
12	6	-4.034654	0.141336	-0.239858
13	1	-4.772261	0.805434	-0.693623

14	6	-2.689200	0.515676	-0.180370
15	6	-0.973343	-2.303382	1.470306
16	1	-0.940659	-2.076563	2.549014
17	1	-1.192114	-3.382057	1.378509
18	6	0.747517	-2.741349	-0.274473
19	1	0.492268	-3.809917	-0.148674
20	1	1.842944	-2.680893	-0.345936
21	6	0.099999	-2.247494	-1.571044
22	1	0.409135	-2.911690	-2.400433
23	1	-0.993994	-2.330114	-1.486938
24	6	-0.601234	-0.188576	-2.730610
25	1	-1.579625	-0.600746	-2.444411
26	1	-0.454639	-0.431418	-3.799842
27	6	-0.614651	1.334082	-2.561756
28	1	0.338721	1.758879	-2.911491
29	1	-1.406877	1.751524	-3.209725
30	6	-2.165195	1.853430	-0.661550
31	1	-2.140917	2.519285	0.219797
32	1	-2.853144	2.288164	-1.407541
33	6	1.791643	-0.684538	-2.409155
34	1	1.826278	0.206255	-3.056272
35	1	2.078301	-1.544040	-3.040675
36	1	-0.322189	2.666847	-1.028966
37	1	1.047282	-2.028363	1.639263
38	1	1.804954	1.611825	1.952428
39	1	1.147502	2.715199	0.967989
40	8	3.171568	0.787427	2.245734
41	8	1.071424	3.948296	-0.257804
42	1	1.876313	4.104260	-0.780051
43	1	0.802187	4.830318	0.049573
44	1	2.906078	-0.036442	2.716292
45	1	3.200030	0.480430	1.301814
46	6	2.882592	-0.464486	-1.341436
47	8	2.464044	0.013265	-0.213274
48	8	4.053978	-0.699200	-1.632695
49	8	2.270152	-1.698837	3.186488
50	1	1.820202	-1.744479	4.047191
51	1	2.974327	-2.366236	3.251021
52	8	-1.501131	3.006592	2.468534
53	1	-2.029581	2.250352	2.768478
54	1	-0.621821	2.605055	2.291229

E(UTPSSh) = -2408.5067531 Hartree
Zero-point correction = 0.449814
Thermal correction to Energy = 0.481322
Thermal correction to Enthalpy = 0.482266
Thermal correction to Gibbs Free Energy = 0.387020
Sum of electronic and zero-point Energies = -2408.056939
Sum of electronic and thermal Energies = -2408.025431
Sum of electronic and thermal Enthalpies = -2408.024487
Sum of electronic and thermal Free Energies = -2408.119733

$[Mn(L3)(H_2O)_2]^+ \cdot 8H_2O$, B3LYP/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1	0.210529	0.138159	-4.251238
2	1	1.360936	-1.994893	-3.830072
3	1	-0.675256	2.506077	-2.886312
4	6	0.593875	-0.057466	-3.232627
5	1	1.585143	0.421837	-3.169358
6	1	-0.240882	-2.054209	-3.066678
7	6	0.746309	-1.564322	-3.017069
8	6	-0.226811	1.964276	-2.033405

9	1	0.829992	2.282686	-1.985702
10	7	-0.268631	0.509854	-2.188429
11	1	2.154646	-3.783967	-1.827523
12	6	-0.909573	2.385120	-0.743451
13	1	0.427730	-3.691646	-1.431455
14	6	1.403218	-3.208976	-1.254738
15	6	1.732014	-3.266935	0.238009
16	1	2.695396	-2.764716	0.428042
17	1	1.855479	-4.320497	0.551531
18	6	-1.389592	1.790789	1.464767
19	1	-2.205420	0.065805	2.444029
20	7	-0.130161	-0.144792	2.291042
21	6	-1.304316	0.699577	2.517543
22	6	0.971500	-2.335677	2.421974
23	1	1.964223	-1.860646	2.498103
24	1	-1.084475	-1.888042	2.943214
25	1	1.023517	-3.273430	3.006644
26	6	-0.092673	-1.416607	3.026131
27	1	-1.323241	1.154516	3.524962
28	1	0.110165	-1.275999	4.104302
29	25	0.124007	-0.550476	-0.071234
30	8	-1.943053	-1.471568	-0.379320
31	8	2.187508	0.385386	0.287248
32	1	-2.495085	-1.054146	-1.095778
33	1	-2.527618	-1.555149	0.416695
34	1	2.419734	1.178772	-0.246476
35	1	2.368586	0.670998	1.228092
36	1	-1.242847	0.244290	-2.382605
37	1	0.706153	0.401102	2.524708
38	7	-0.856551	1.504990	0.267457
39	6	-2.013659	3.020131	1.700129
40	6	-1.529729	3.628013	-0.586143
41	6	-2.085628	3.944161	0.655705
42	1	-2.435103	3.244551	2.681913
43	1	-2.572871	4.909845	0.809502
44	1	-1.573847	4.331782	-1.419626
45	8	2.558647	1.401239	2.699086
46	8	3.586581	2.234744	-1.172746
47	8	-3.255607	-2.271512	1.847338
48	8	-3.163982	-0.164004	-2.334178
49	1	2.990905	2.216138	2.317529
50	1	3.248549	0.976604	3.231031
51	1	3.473732	2.775505	-1.968151
52	1	4.059548	1.416099	-1.455311
53	1	-2.972566	-3.159248	1.536821
54	1	-4.223859	-2.294239	1.836583
55	1	-3.686445	-0.611246	-3.015207
56	1	-3.734425	0.566172	-1.973274
57	7	0.682916	-2.578031	1.002220
58	7	1.318932	-1.809001	-1.688781
59	1	-0.165866	-3.152040	0.934285
60	1	2.264830	-1.412970	-1.675851
61	8	-1.877055	-4.106112	0.348680
62	1	-2.078179	-4.921196	-0.133051
63	1	-1.952916	-3.374182	-0.299138
64	8	4.183257	-0.405806	-1.384116
65	1	3.693434	-0.375411	-0.535110
66	1	5.001204	-0.892600	-1.204913
67	8	3.755711	3.392721	1.372093
68	1	3.834631	3.057311	0.451692
69	1	3.210531	4.189190	1.288900
70	8	-4.533918	1.819873	-1.180160
71	1	-5.478551	1.669491	-1.023251
72	1	-4.500168	2.662093	-1.658559

E(UB3LYP) = -2697.0180428 Hartree
Zero-point correction = 0.622616

Thermal correction to Energy = 0.667139
Thermal correction to Enthalpy = 0.668083
Thermal correction to Gibbs Free Energy = 0.544152
Sum of electronic and zero-point Energies = -2696.395427
Sum of electronic and thermal Energies = -2696.350904
Sum of electronic and thermal Enthalpies = -2696.349960
Sum of electronic and thermal Free Energies = -2696.473891

$[Mn(L3)(H_2O)_2]^+ \cdot 8H_2O$, TPSSh/SVP (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1	0.072381	0.192846	4.233810
2	1	-1.014501	-2.004658	3.915034
3	1	0.749977	2.556153	2.803824
4	6	-0.374010	-0.043279	3.250807
5	1	-1.389112	0.386825	3.244579
6	1	0.546528	-2.000975	3.065088
7	6	-0.462964	-1.557723	3.067380
8	6	0.264246	1.994016	1.986140
9	1	-0.807418	2.259025	2.013959
10	7	0.385047	0.541604	2.135372
11	1	-1.808306	-3.858672	2.001414
12	6	0.831020	2.435956	0.650974
13	1	-0.120542	-3.674301	1.472863
14	6	-1.134287	-3.255242	1.366393
15	6	-1.570875	-3.343214	-0.094993
16	1	-2.565564	-2.883461	-0.216354
17	1	-1.662450	-4.402193	-0.398287
18	6	1.170508	1.846951	-1.584852
19	1	1.993995	0.158988	-2.617237
20	7	-0.043509	-0.160110	-2.283789
21	6	1.058392	0.744849	-2.620475
22	6	-1.022927	-2.404404	-2.330952
23	1	-2.042747	-1.985385	-2.332345
24	1	0.959705	-1.844175	-3.011325
25	1	-1.062691	-3.353489	-2.896445
26	6	-0.062358	-1.434488	-3.018723
27	1	0.962343	1.188123	-3.628009
28	1	-0.357148	-1.306552	-4.076364
29	25	-0.087518	-0.552395	0.075246
30	8	2.040111	-1.340071	0.221092
31	8	-2.223094	0.255468	-0.133637
32	1	2.610438	-0.903591	0.920137
33	1	2.584676	-1.372946	-0.614009
34	1	-2.446367	1.070159	0.380375
35	1	-2.497383	0.492319	-1.073257
36	1	1.384981	0.322150	2.267552
37	1	-0.929344	0.334348	-2.455071
38	7	0.738763	1.543276	-0.349294
39	6	1.721336	3.100996	-1.871238
40	6	1.386759	3.702497	0.444245
41	6	1.832801	4.035001	-0.838081
42	1	2.058327	3.335796	-2.882500
43	1	2.265906	5.018761	-1.031270
44	1	1.464292	4.411659	1.270273
45	8	-2.853445	1.138944	-2.529548
46	8	-3.633461	2.097274	1.288995

47	8	3.278704	-2.041079	-2.054338
48	8	3.285637	-0.054002	2.157622
49	1	-3.329866	1.942843	-2.158294
50	1	-3.540062	0.635706	-2.997571
51	1	-3.496411	2.672504	2.058824
52	1	-4.037249	1.259333	1.635236
53	1	3.058585	-2.944653	-1.723380
54	1	4.248946	-2.007579	-2.065841
55	1	3.793918	-0.542586	2.824267
56	1	3.867409	0.704339	1.861625
57	7	-0.612798	-2.604908	-0.932835
58	7	-1.095783	-1.843345	1.772590
59	1	0.269055	-3.137313	-0.925639
60	1	-2.063166	-1.497943	1.813843
61	8	2.089888	-3.938986	-0.512081
62	1	2.388509	-4.721073	-0.021523
63	1	2.147882	-3.180463	0.116068
64	8	-4.054280	-0.537557	1.673046
65	1	-3.578899	-0.508586	0.808535
66	1	-4.861948	-1.051782	1.511666
67	8	-4.113474	3.106480	-1.257625
68	1	-4.071590	2.818863	-0.313596
69	1	-3.613654	3.939187	-1.271537
70	8	4.713570	1.999834	1.247247
71	1	5.650890	1.793167	1.094755
72	1	4.736498	2.741611	1.874721

E(UTPSSh) = -2697.0298537 Hartree

Zero-point correction = 0.620865
Thermal correction to Energy = 0.664999
Thermal correction to Enthalpy = 0.665943
Thermal correction to Gibbs Free Energy = 0.542383
Sum of electronic and zero-point Energies = -2696.408989
Sum of electronic and thermal Energies = -2696.364855
Sum of electronic and thermal Enthalpies = -2696.363911
Sum of electronic and thermal Free Energies = -2696.487470

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