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Making a next step toward inert Mn^{2+} complexes of open-chain ligands: the case of the rigid PhDTA‡ ligand†

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Electronic Supporting Information

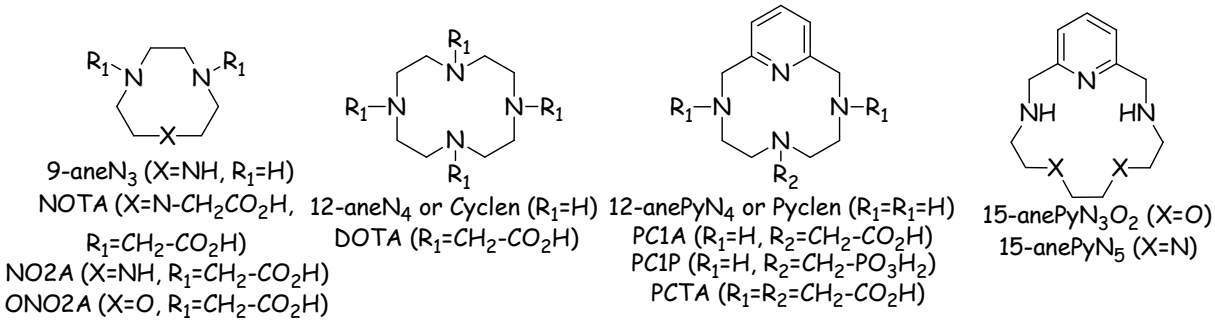

Figure S1. Structures of the ligands mentioned in the text.

Table S1. Experimental (X-ray) and calculated (DFT) bond distances (Å) of the metal coordination environments in $[Mn(PhDTA)(H_2O)]^{2-}$ and $[Mn(EDTA)(H_2O)]^{2-}$.

	PhDTA (X-ray)	PhDTA (DFT)	EDTA (DFT)
Mn-N1	2.403	2.439	2.415
Mn-N2	2.429	2.440	2.406
Mn-O2	2.250	2.234	2.271
Mn-O3	2.200	2.222	2.222
Mn-O5	2.218	2.234	2.292
Mn-O7	2.175	2.168	2.187
Mn-O11	2.242	2.273	2.251

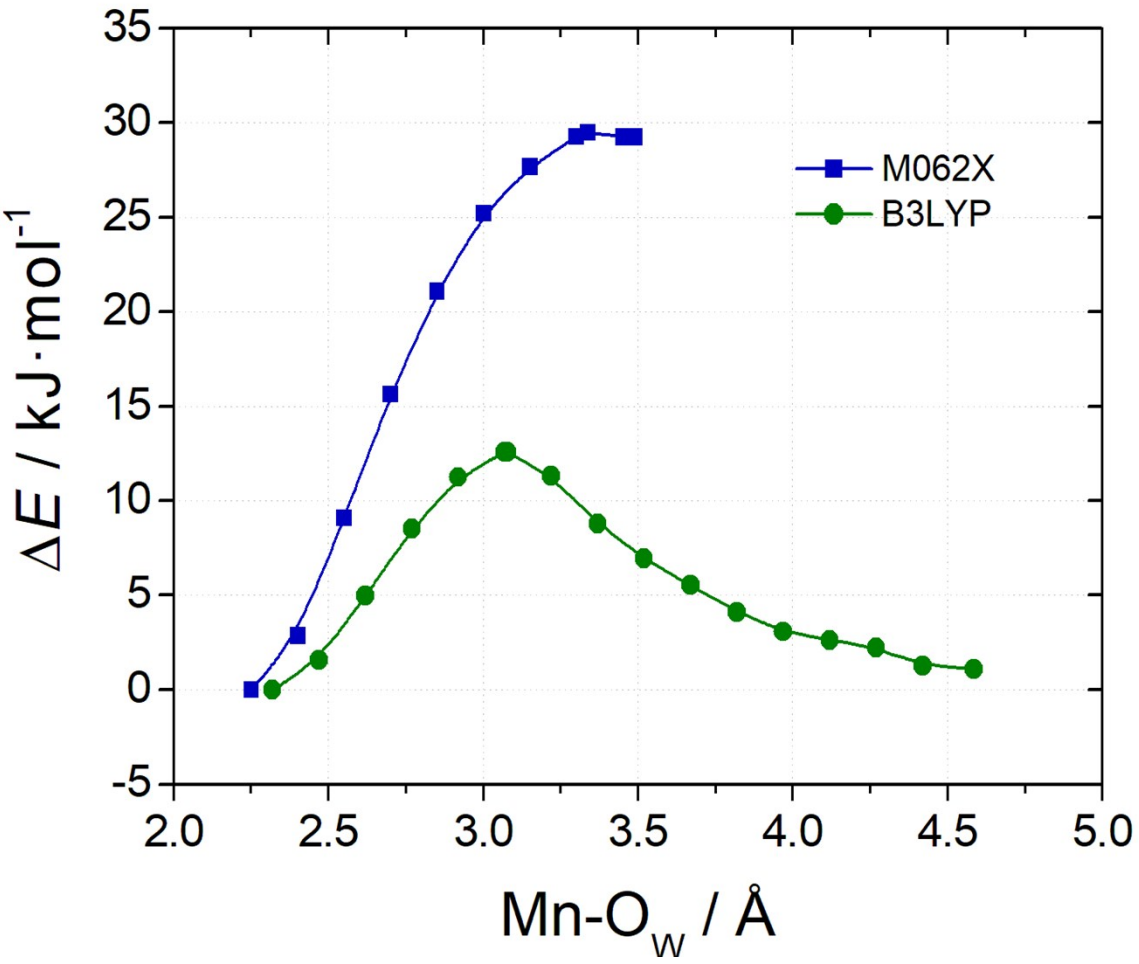

Figure S2. Relaxed potential energy surface scans calculated for $[Mn(EDTA)(H_2O)]^{2-}\cdot 2H_2O$ using different functionals.

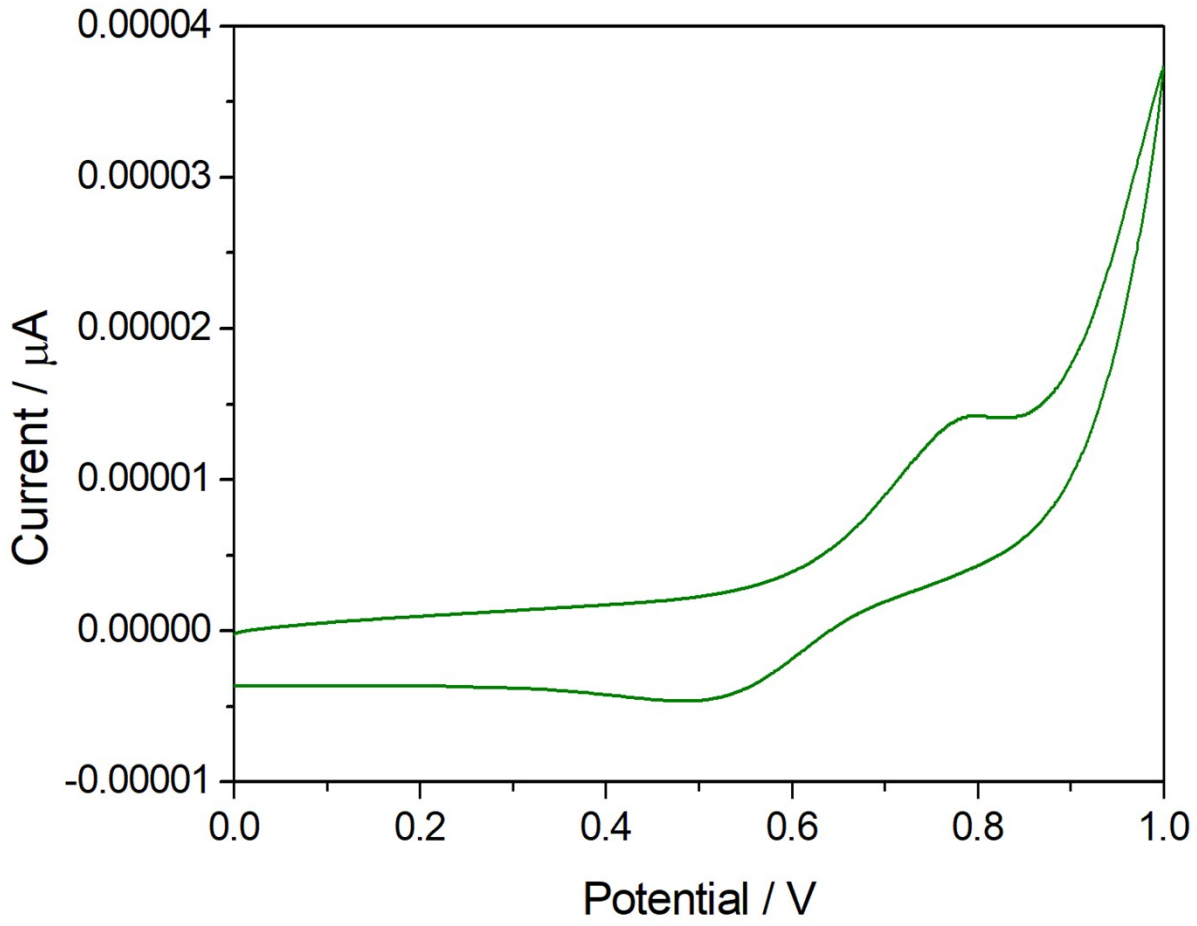

Figure S3. Cyclic voltammograms recorded for 3 mM $[Mn(EDTA)]^{2-}$ (pH = 7.1, 0.15 NaCl, scan rate 50 mV/s, potentials reported vs Ag/AgCl).

Table S2. $[Mn(PhDTA)(H_2O)]^{-}\cdot 2H_2O$, M062X/tzvp, aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.987306	-0.988840	1.367426
2	7	0	1.716890	-1.177529	0.416948
3	8	0	-0.466939	2.095634	-1.709741
4	8	0	-2.288884	0.099274	-0.714718
5	8	0	1.944253	0.935744	-1.189560
6	8	0	3.641993	1.844989	-0.069669
7	8	0	-4.059546	-1.237124	-0.475085
8	6	0	2.797793	0.952326	-0.260187
9	8	0	0.221896	1.475250	1.211691
10	6	0	-2.908659	-0.892835	-0.205869
11	8	0	-0.080279	-1.729393	-1.606130
12	8	0	-0.294211	1.905543	3.340217
13	6	0	-0.400393	1.252539	2.301749
14	8	0	0.962844	-3.654304	-2.037385
15	6	0	0.892452	-2.540959	-1.507101
16	6	0	2.762497	-0.203241	0.750434

17	6	0	-1.414276	0.101966	2.256618
18	6	0	-2.131457	-1.727420	0.821509
19	6	0	2.104299	-2.049204	-0.701268
20	6	0	1.283925	-1.937422	1.561129
21	6	0	-0.032255	-1.854173	2.017983
22	1	0	-1.753556	-2.607013	0.296914
23	1	0	3.759684	-0.655932	0.809107
24	1	0	2.707063	-1.456914	-1.392599
25	1	0	-2.831314	-2.060385	1.595324
26	1	0	-1.623399	-0.243358	3.271999
27	1	0	2.699517	-2.906029	-0.375350
28	1	0	-1.373882	2.451669	-1.668579
29	1	0	0.147719	2.748224	-1.322479
30	1	0	-2.332493	0.532798	1.849469
31	1	0	2.532379	0.234744	1.721676
32	8	0	-3.209327	2.434063	-1.556493
33	1	0	-3.711824	2.418701	-2.376092
34	1	0	-3.071139	1.492476	-1.294880
35	8	0	1.282610	3.639316	-0.073819
36	1	0	0.932876	2.977831	0.560149
37	1	0	2.163297	3.287245	-0.282663
38	25	0	-0.061157	0.172881	-0.566601
39	6	0	-0.419118	-2.614652	3.124739
40	6	0	2.187149	-2.765615	2.232697
41	6	0	0.480844	-3.438142	3.778089
42	1	0	0.160381	-4.018973	4.633403
43	6	0	1.796616	-3.509979	3.331548
44	1	0	2.513173	-4.143138	3.838835
45	1	0	3.210707	-2.821056	1.880539
46	1	0	-1.442364	-2.551526	3.476124

E(UM062X) = -2632.8798453 Hartree
Zero-point correction = 0.339638 (/Particle)
Thermal correction to Energy = 0.368886
Thermal correction to Enthalpy = 0.369830
Thermal correction to Gibbs Free Energy = 0.278980
Sum of electronic and zero-point Energies = -2632.540207
Sum of electronic and thermal Energies = -2632.510960
Sum of electronic and thermal Enthalpies = -2632.510015
Sum of electronic and thermal Free Energies = -2632.600865

Table S3. $[Mn(PhDTA)]^{-}\cdot 3H_2O$, M062X/tzvp, aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.719706	1.327690	-0.632206
2	7	0	1.168663	-1.319311	0.412666
3	8	0	-4.762277	-0.516857	0.407585
4	8	0	-1.339623	2.140259	0.909755
5	8	0	-1.330663	-1.973590	1.137366
6	8	0	-1.343807	-3.877299	-0.022033
7	8	0	-0.520724	4.204973	1.111797
8	6	0	-0.807202	-2.827445	0.360047
9	8	0	-1.325615	-0.373649	-1.303530
10	6	0	-0.427353	3.029930	0.769653
11	8	0	0.621480	0.471015	2.423113
12	8	0	-1.105325	0.132810	-3.465280
13	6	0	-0.879558	0.328851	-2.273021
14	8	0	2.412930	-0.206026	3.571316
15	6	0	1.582046	-0.325190	2.666755
16	6	0	0.595179	-2.524217	-0.197269
17	6	0	-0.046958	1.551369	-1.868821
18	6	0	0.895185	2.569928	0.131202
19	6	0	1.661414	-1.573599	1.775400
20	6	0	2.161734	-0.668057	-0.405543

21	6	0	1.956724	0.627764	-0.888798
22	1	0	1.593390	2.376943	0.947218
23	1	0	1.228199	-3.408380	-0.063376
24	1	0	1.006116	-2.317065	2.234762
25	1	0	1.287415	3.390189	-0.477976
26	1	0	0.586981	1.857629	-2.703774
27	1	0	2.680016	-1.968209	1.782582
28	1	0	-4.440687	0.372397	0.182259
29	1	0	-4.320698	-1.129250	-0.206505
30	1	0	-0.768943	2.351551	-1.683616
31	1	0	0.475262	-2.353053	-1.267667
32	8	0	-3.840018	2.113796	-0.122296
33	1	0	-4.393952	2.830483	0.200430
34	1	0	-2.962990	2.237273	0.299503
35	8	0	-3.334062	-2.229222	-1.364352
36	1	0	-2.606130	-1.576798	-1.460301
37	1	0	-2.917195	-2.954574	-0.872101
38	25	0	-0.722813	0.065751	0.763163
39	6	0	2.959430	1.239377	-1.644089
40	6	0	3.352479	-1.329266	-0.713193
41	6	0	4.141583	0.579622	-1.932487
42	1	0	4.907006	1.072924	-2.517525
43	6	0	4.335904	-0.718137	-1.471094
44	1	0	5.251257	-1.248776	-1.699056
45	1	0	3.503169	-2.337361	-0.344694
46	1	0	2.801537	2.246368	-2.012432

E(UM062X) = -2632.8707371 Hartree
Zero-point correction = 0.338493
Thermal correction to Energy = 0.368331
Thermal correction to Enthalpy = 0.369275
Thermal correction to Gibbs Free Energy = 0.276282
Sum of electronic and zero-point Energies = -2632.532245
Sum of electronic and thermal Energies = -2632.502406
Sum of electronic and thermal Enthalpies = -2632.501462
Sum of electronic and thermal Free Energies = -2632.594456

Table S4. $[Mn(PhDTA)(H_2O)]^{-}\cdot 2H_2O$, B3LYP/tzvp, aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.567300	-1.412103	-0.628287
2	7	0	-1.332926	1.167424	0.464228
3	8	0	3.227212	0.700347	0.666528
4	8	0	1.807456	-1.903111	0.619170
5	8	0	1.033128	2.402597	0.768338
6	8	0	0.533593	4.114825	-0.581705
7	8	0	1.322080	-4.068191	0.935586
8	6	0	0.258584	3.044177	-0.001525
9	8	0	1.154638	0.535567	-1.636044
10	6	0	1.021180	-2.913616	0.607995
11	8	0	0.015004	-0.258875	2.451724
12	8	0	0.823184	-0.163087	-3.738760
13	6	0	0.707108	-0.281818	-2.511779
14	8	0	-1.590277	0.196854	3.945532
15	6	0	-1.035318	0.347448	2.844865
16	6	0	-1.122215	2.424007	-0.283855
17	6	0	0.032170	-1.555340	-1.974000
18	6	0	-0.429533	-2.647854	0.168720
19	6	0	-1.625217	1.405340	1.893771
20	6	0	-2.307911	0.301838	-0.163406
21	6	0	-1.940034	-0.944842	-0.687759
22	1	0	-1.021574	-2.535420	1.078130
23	1	0	-1.896854	3.172307	-0.077395
24	1	0	-1.160734	2.349903	2.179927

25	1	0	-0.795787	-3.534095	-0.359485
26	1	0	-0.690405	-1.911844	-2.711019
27	1	0	-2.696510	1.497339	2.085985
28	1	0	3.826233	-0.038974	0.437745
29	1	0	3.332506	1.398011	-0.009585
30	1	0	0.825546	-2.303409	-1.917127
31	1	0	-1.161091	2.202777	-1.349939
32	8	0	4.452508	-1.773926	0.281026
33	1	0	4.970273	-2.097409	1.026508
34	1	0	3.511484	-2.018422	0.472702
35	8	0	3.019357	2.553053	-1.574140
36	1	0	2.364021	1.855483	-1.802297
37	1	0	2.461768	3.249306	-1.188015
38	25	0	0.936478	0.169820	0.542938
39	6	0	-2.923837	-1.749798	-1.276480
40	6	0	-3.644295	0.710637	-0.260429
41	6	0	-4.244747	-1.337090	-1.358655
42	1	0	-4.985055	-1.980638	-1.817437
43	6	0	-4.607656	-0.092411	-0.850493
44	1	0	-5.633464	0.248962	-0.913071
45	1	0	-3.928188	1.677068	0.137211
46	1	0	-2.645305	-2.716192	-1.677726

E(UB3LYP) = -2633.4499928 Hartree
Zero-point correction = 0.333639
Thermal correction to Energy = 0.363931
Thermal correction to Enthalpy = 0.364875
Thermal correction to Gibbs Free Energy = 0.270752
Sum of electronic and zero-point Energies = -2633.116354
Sum of electronic and thermal Energies = -2633.086062
Sum of electronic and thermal Enthalpies = -2633.085117
Sum of electronic and thermal Free Energies = -2633.179241

Table S5. $[Mn(PhDTA)]^{-}\cdot 3H_2O$, B3LYP/tzvp, aqueous solution (0 Imaginary Frequencies)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.817049	1.339274	-0.657492
2	7	0	1.237603	-1.328326	0.421565
3	8	0	-5.110054	-0.652437	0.131568
4	8	0	-1.355109	2.109487	0.813872
5	8	0	-1.334583	-1.989101	0.940598
6	8	0	-1.288208	-3.850102	-0.300729
7	8	0	-0.609652	4.215756	0.989526
8	6	0	-0.762594	-2.824680	0.169447
9	8	0	-1.326508	-0.246371	-1.450522
10	6	0	-0.464915	3.027645	0.689059
11	8	0	0.444720	0.347649	2.488104
12	8	0	-1.126391	0.398592	-3.587563
13	6	0	-0.838198	0.476139	-2.387244
14	8	0	2.042043	-0.443740	3.846326
15	6	0	1.372902	-0.468371	2.802096
16	6	0	0.687479	-2.517436	-0.264364
17	6	0	0.143994	1.578180	-1.957920
18	6	0	0.908958	2.580956	0.142937
19	6	0	1.635965	-1.623415	1.817574
20	6	0	2.279777	-0.647053	-0.321322
21	6	0	2.087563	0.652957	-0.815303
22	1	0	1.546614	2.385902	1.006105
23	1	0	1.301200	-3.411507	-0.110842
24	1	0	1.029864	-2.459051	2.171081
25	1	0	1.345165	3.411441	-0.419528
26	1	0	0.862307	1.744546	-2.761931
27	1	0	2.681766	-1.927694	1.890402
28	1	0	-4.689188	0.215064	0.275176

29	1	0	-4.510956	-1.156297	-0.453133
30	1	0	-0.453989	2.487869	-1.874578
31	1	0	0.660683	-2.320542	-1.335713
32	8	0	-4.075962	1.983377	0.669730
33	1	0	-4.469845	2.338365	1.474252
34	1	0	-3.105798	2.127064	0.766339
35	8	0	-3.355106	-2.111219	-1.599389
36	1	0	-2.648491	-1.427845	-1.665633
37	1	0	-2.908255	-2.840081	-1.135294
38	25	0	-0.683212	0.048904	0.653811
39	6	0	3.139226	1.285345	-1.488523
40	6	0	3.507036	-1.282087	-0.544071
41	6	0	4.354822	0.649793	-1.690390
42	1	0	5.152467	1.162273	-2.213404
43	6	0	4.537218	-0.648458	-1.221971
44	1	0	5.476555	-1.162912	-1.381499
45	1	0	3.654060	-2.289129	-0.173864
46	1	0	2.996672	2.291099	-1.863922

E(UB3LYP) = -2633.4524597 Hartree
Zero-point correction = 0.332875 (Hartree/Particle)
Thermal correction to Energy = 0.363572
Thermal correction to Enthalpy = 0.364516
Thermal correction to Gibbs Free Energy = 0.268332
Sum of electronic and zero-point Energies = -2633.119584
Sum of electronic and thermal Energies = -2633.088888
Sum of electronic and thermal Enthalpies = -2633.087944
Sum of electronic and thermal Free Energies = -2633.184128

Table S6. $[Mn(EDTA)(H_2O)]^{-}\cdot 2H_2O$, M062X/tzvp, aqueous solution (0 Imaginary Frequencies)

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	2.30885800	0.15270700	-0.58973500
O	3.94557700	1.47782000	0.15196400
O	0.72990500	-3.26266800	2.25058200
O	-0.01550100	-2.01493500	0.55679800
O	0.07488300	1.99616800	-1.22250100
O	-1.01896300	3.93248900	-1.41984600
O	-2.03919800	-0.75652200	-1.18506100
O	-3.95717300	-1.46743700	-0.29090400
N	-1.65078200	1.11285200	0.68397500
N	0.94013500	0.27368000	1.68636900
C	-1.08102900	1.68186300	1.90880300
H	-0.54075500	2.58893600	1.62923500
H	-1.86676100	1.98429800	2.61320900
C	-0.12958700	0.70992500	2.58911800
H	-0.67724600	-0.18213800	2.90127900
H	0.27734500	1.16716600	3.50048000
C	1.98964800	1.26843300	1.49455400
H	1.53601500	2.24601900	1.31596100
H	2.64866400	1.35745500	2.36646000
C	2.83810200	0.94807000	0.25439100
C	1.48873600	-1.01175200	2.11654100
H	2.48081700	-1.14189800	1.67853900
H	1.59854000	-1.06964400	3.20472700
C	0.65726900	-2.20468400	1.62207900
C	-2.08552900	2.17094400	-0.22571100
H	-2.76119900	1.74091800	-0.96848400
H	-2.62443700	2.96809400	0.29792400
C	-0.91046000	2.77029800	-1.01432200
C	-2.71385600	0.14637100	0.92767200
H	-2.43166500	-0.50736600	1.75553300
H	-3.66246000	0.62676500	1.19721200
C	-2.93870700	-0.76854400	-0.28596900

O	0.49616400	-1.15592400	-2.45655100
H	1.44038000	-1.26402000	-2.68851500
H	0.08387400	-2.03774800	-2.39773900
O	-1.10250400	-3.28771500	-1.62699600
O	3.23131900	-1.08563200	-2.71135400
H	-0.69202700	-3.13936200	-0.75284000
H	-1.72449200	-2.53590900	-1.65975400
H	3.62382000	-0.51853300	-3.38123400
H	3.08944700	-0.52279100	-1.90868400
Mn	0.05048800	-0.07833300	-0.53079300

E(UM062X) =-2480.4660108 Hartree
Zero-point correction = 0.316987
Thermal correction to Energy = 0.343951
Thermal correction to Enthalpy = 0.344895
Thermal correction to Gibbs Free Energy = 0.258706
Sum of electronic and zero-point Energies = -2480.149023
Sum of electronic and thermal Energies = -2480.122060
Sum of electronic and thermal Enthalpies = -2480.121116
Sum of electronic and thermal Free Energies = -2480.207305

Table S7. $[Mn(EDTA)]^{-}\cdot 3H_2O$, M062X/tzvp, aqueous solution (0 Imaginary Frequencies)

Atom	Coordinates (Angstroms) X	Y	Z
O	-2.11485300	-0.57930700	-0.48726900
O	-3.31098500	-2.41855300	-0.08288000
O	-1.38983300	2.37732600	2.96446900
O	-0.43742500	1.75366700	1.04479400
O	0.38236000	-1.67394700	-1.54435800
O	1.92138600	-3.12876900	-2.25184800
O	1.59377200	1.44560900	-1.05420300
O	3.36073500	2.51625500	-0.21125500
N	2.00759300	-0.74678300	0.41524300
N	-0.60250900	-0.88605300	1.67925400
C	1.74155300	-1.68058500	1.51570500
H	1.45637400	-2.63498200	1.06733000
H	2.64365400	-1.86725100	2.11165500
C	0.62400000	-1.19083000	2.42472700
H	0.93456600	-0.26988000	2.92342000
H	0.44272300	-1.93339200	3.21194200
C	-1.36318200	-2.05330800	1.24372400
H	-0.68351400	-2.78880300	0.80784000
H	-1.90622700	-2.53586800	2.06400000
C	-2.36144600	-1.67003700	0.13643500
C	-1.43881600	0.06611800	2.41016600
H	-2.47275600	-0.02870200	2.07147500
H	-1.42960300	-0.12209500	3.48820400
C	-1.05041500	1.52740800	2.14092600
C	2.61079500	-1.43910900	-0.72308700
H	3.07834300	-0.70188600	-1.37946100
H	3.38508600	-2.14707100	-0.41007400
C	1.55592400	-2.16228900	-1.57641100
C	2.76179100	0.44364300	0.78976100
H	2.38619200	0.83184700	1.73949700
H	3.83247200	0.24428400	0.91282300
C	2.57517500	1.56959300	-0.24419600
O	-1.46641900	1.93340700	-2.99863800
H	-2.31892500	1.56555700	-2.70844200
H	-1.16219100	2.52804900	-2.29105500
O	-0.18288900	3.53023700	-1.03309000
O	-3.82417000	0.66934800	-2.08443800
H	-0.42812300	3.15882400	-0.16523100
H	0.61954400	3.01011600	-1.22926700
H	-4.26515200	0.07018200	-2.69335200

H	-3.28198500	0.10115500	-1.48354400
Mn	-0.03407100	0.12335800	-0.37984000

E(UM062X) = -2480.4548727 Hartree
Zero-point correction = 0.315845
Thermal correction to Energy = 0.343403
Thermal correction to Enthalpy = 0.344347
Thermal correction to Gibbs Free Energy = 0.255518
Sum of electronic and zero-point Energies = -2480.139028
Sum of electronic and thermal Energies = -2480.111470
Sum of electronic and thermal Enthalpies = -2480.110525
Sum of electronic and thermal Free Energies = -2480.199355

Table S8. $[Mn(EDTA)(H_2O)]^{-}\cdot 2H_2O$, B3LYP/tzvp, aqueous solution (0 Imaginary Frequencies)

Atom	Coordinates (Angstroms) X	Y	Z
O	-2.27174600	-0.49211100	-0.63321100
O	-3.81026800	-1.91463200	0.16875500
O	-1.36768800	3.23527800	2.09136600
O	-0.44786400	2.04723800	0.42940600
O	0.28110600	-1.91928900	-1.32383200
O	1.57950400	-3.73413900	-1.53274100
O	1.98737800	1.09143500	-1.00910900
O	3.92871700	1.81681100	-0.15168700
N	1.79369000	-0.95029100	0.76473600
N	-0.95117500	-0.35537000	1.71657600
C	1.22332000	-1.55970600	1.97901200
H	0.78646600	-2.51780800	1.69411800
H	2.00284000	-1.78304300	2.72017000
C	0.15977300	-0.68219000	2.63021100
H	0.60805000	0.25985000	2.94892600
H	-0.20367600	-1.17740800	3.54102500
C	-1.89357700	-1.46324700	1.52006900
H	-1.33780700	-2.39365600	1.39051100
H	-2.55706400	-1.60146300	2.38221300
C	-2.74902400	-1.28077700	0.25220400
C	-1.64780500	0.87034700	2.14268000
H	-2.69076600	0.81581500	1.82487100
H	-1.65912500	0.97147400	3.23261000
C	-1.09830800	2.16766500	1.52178700
C	2.35880200	-1.97132000	-0.12973200
H	3.09367400	-1.49638600	-0.78309200
H	2.88523600	-2.75475200	0.42638500
C	1.31755600	-2.61423400	-1.06438400
C	2.76406900	0.11303600	1.04058600
H	2.41857500	0.71180900	1.88568100
H	3.74830000	-0.28502000	1.31530300
C	2.92503800	1.08720600	-0.14281900
O	-0.51830200	1.02644900	-2.57020600
H	-1.47299800	1.00879100	-2.79593200
H	-0.24316400	1.96231800	-2.49097200
O	0.67929300	3.40956700	-1.69176100
O	-3.24938100	0.61583900	-2.82961600
H	0.18096700	3.24518200	-0.86434500
H	1.39983100	2.75138600	-1.59212700
H	-3.52100000	-0.02214800	-3.49869300
H	-3.06485700	0.09149200	-2.00549200
Mn	-0.03024500	0.07571800	-0.51107700

E(UB3LYP) = -2480.987866 Hartree
Zero-point correction = 0.311551
Thermal correction to Energy = 0.339190
Thermal correction to Enthalpy = 0.340135

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 Thermal correction to Gibbs Free Energy = 0.252092
 Sum of electronic and zero-point Energies = -2480.676315
 Sum of electronic and thermal Energies = -2480.648676
 Sum of electronic and thermal Enthalpies = -2480.647731
 Sum of electronic and thermal Free Energies = -2480.735774
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Table S9. $[Mn(EDTA)]^{-}\cdot 3H_2O$, B3LYP/tzvp, aqueous solution (0 Imaginary Frequencies)

Atom	Coordinates (Angstroms) X	Y	Z
O	-1.78183800	-1.19241100	-0.65007900
O	-2.40154100	-3.34664000	-0.56832900
O	-2.03255300	1.04341200	3.36843600
O	-1.02022700	1.17538400	1.37370200
O	0.81027500	-0.92509900	-2.00866200
O	2.64892000	-1.62981600	-3.07912400
O	1.03678700	2.05259600	-0.57394900
O	2.61096800	3.35445700	0.35133600
N	2.24577700	-0.23093500	0.24155600
N	-0.14411900	-1.43807000	1.48867300
C	2.33287300	-1.42005300	1.11136500
H	2.31729400	-2.29769200	0.46381000
H	3.28609900	-1.45161900	1.65509700
C	1.18941200	-1.50578900	2.11904500
H	1.25576200	-0.67187800	2.81905700
H	1.30767800	-2.42218800	2.71195500
C	-0.56461200	-2.66766300	0.80321100
H	0.27840900	-3.07673600	0.24292400
H	-0.89664200	-3.44288600	1.50265500
C	-1.68986900	-2.39859000	-0.22054800
C	-1.16855400	-0.97146400	2.44058800
H	-2.12559400	-1.43426300	2.19304200
H	-0.93367100	-1.27581700	3.46452800
C	-1.42270900	0.54714800	2.41222100
C	2.95125900	-0.44515900	-1.03438600
H	3.27380800	0.52117300	-1.42673300
H	3.85434500	-1.04850200	-0.90070900
C	2.07109200	-1.07135300	-2.13367800
C	2.65705900	1.02622800	0.87871000
H	2.28186700	1.05516800	1.90386000
H	3.74675500	1.12820400	0.93229500
C	2.06883100	2.25932300	0.15693100
O	-3.27205000	2.76584500	-2.18640700
H	-3.38403800	1.79663300	-2.16934600
H	-2.61366400	2.97390100	-1.49432800
O	-1.35868000	3.42318900	-0.18562100
O	-3.67185300	-0.06668600	-2.21544100
H	-1.45784400	2.76825000	0.53574600
H	-0.45940900	3.20094900	-0.50012700
H	-3.59425900	-0.43908300	-3.10068900
H	-3.01179100	-0.55815300	-1.66460400
Mn	-0.03724300	0.12031800	-0.29950700

```
E(UB3LYP) = -2480.9874482 Hartree
Zero-point correction = 0.310545
 Thermal correction to Energy = 0.338761
 Thermal correction to Enthalpy = 0.339705
 Thermal correction to Gibbs Free Energy = 0.248225
 Sum of electronic and zero-point Energies = -2480.676903
 Sum of electronic and thermal Energies =             -2480.648687
 Sum of electronic and thermal Enthalpies = -2480.647743
 Sum of electronic and thermal Free Energies = -2480.739223
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