

Supplementary Information

Mechanistic Insights into Dioxygen Activation by a Manganese Corrole Complex: A Broken-Symmetry DFT Study

Jiangfeng Yu, Wenzhen Lai*

Department of Chemistry, Renmin University of China, Beijing, 100872, China.

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Part I. Dioxygen Binding of Mn(III) Corrole Complex

A. Without the axial OH⁻ ligand.

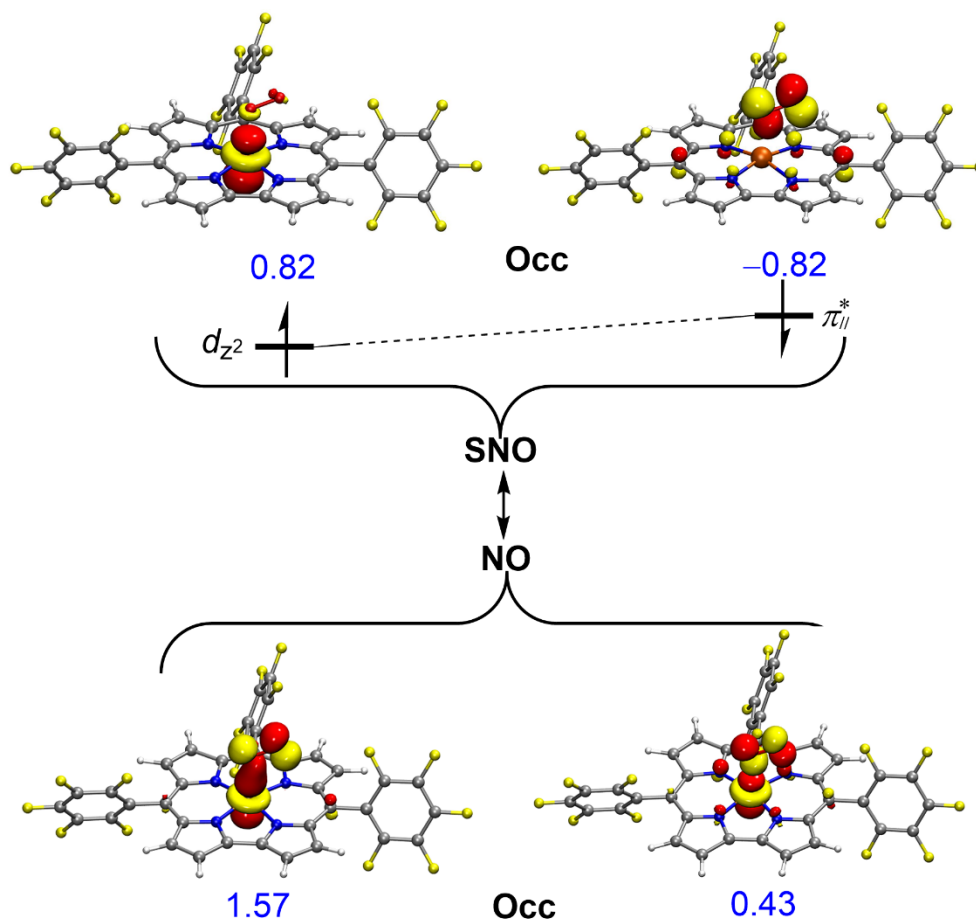


Fig. S1 Spin natural orbitals (SNO) and natural orbitals (NO) responsible for Mn-O₂ bonding in the quintet [(TPFC)MnO₂].

Table S1. The calculated expectation values of $\langle S^2 \rangle$ and absolute energies (in Hartree) of [(TPFC)Mn^{III}(O₂)].

species	septet	quintet	triplet	singlet
$\langle S^2 \rangle$	12.0321	6.2610	2.9167	0.0000
<i>E</i> (BP86/def2-SVP)	-4430.361923	-4430.364162	-4430.377081	-4430.368495
<i>E</i> (BP86/def2-TZVP)	-4434.246159	-4434.247586	-4434.260499	-4434.252117
<i>E</i> (DKH2-BP86)	-4443.935531	-4443.937640	-4443.951203	-4443.943754
ZPE(BP86/def2-SVP)	0.368264	0.368769	0.369449	0.371922
<i>H</i> _{corr} (BP86/def2-SVP)	0.419712	0.419446	0.419752	0.421593
<i>G</i> _{corr} (BP86/def2-SVP)	0.276546	0.280156	0.282995	0.286134
<i>E</i> _{disp}	-0.102346	-0.106632	-0.107075	-0.105842
<i>H</i> (BP86-D3)	-4443.618165	-4443.624826	-4443.638526	-4443.628003
<i>G</i> (BP86-D3)	-4443.761331	-4443.764116	-4443.775283	-4443.763462
$\langle S^2 \rangle$	12.0405	6.7087	3.8380	1.8628
<i>E</i> (TPSSh/def2-SVP)	-4430.264358	-4430.252049	-4430.262526	-4430.232936
<i>E</i> (TPSSh/def2-TZVP)	-4434.134052	-4434.120315	-4434.129832	-4434.101082
<i>E</i> (DKH2-TPSSh)	-4443.729611	-4443.716184	-4443.725558	-4443.696404
ZPE(TPSSh/def2-SVP)	0.378790	0.378790	0.378653	0.378754
<i>H</i> _{corr} (TPSSh/def2-SVP)	0.429113	0.428552	0.427841	0.427984
<i>G</i> _{corr} (TPSSh/def2-SVP)	0.288883	0.291635	0.292830	0.294830
<i>E</i> _{disp}	-0.075989	-0.078089	-0.078002	-0.078369
<i>H</i> (TPSSh-D3)	-4443.376487	-4443.390834	-4443.400093	-4443.372746
<i>G</i> (TPSSh-D3)	-4443.516717	-4443.502638	-4443.510730	-4443.479943
$\langle S^2 \rangle$	12.0449	6.9403	4.0196	2.0606
<i>E</i> (B3LYP/def2-SVP)	-4430.137344	-4430.119108	-4430.134498	-4430.098642
<i>E</i> (B3LYP/def2-TZVP)	-4434.051191	-4434.030792	-4434.046916	-4434.009346
<i>E</i> (DKH2-B3LYP)	-4443.699161	-4443.678732	-4443.694825	-4443.656578
ZPE(B3LYP/def2-SVP)	0.380858	0.380409	0.380663	0.380278
<i>H</i> _{corr} (B3LYP/def2-SVP)	0.430593	0.430103	0.430569	0.429156
<i>G</i> _{corr} (B3LYP/def2-SVP)	0.292118	0.291625	0.291370	0.296505
<i>E</i> _{disp}	-0.092164	-0.094218	-0.093353	-0.094513
<i>H</i> (B3LYP-D3)	-4443.360732	-4443.342847	-4443.357609	-4443.321935
<i>G</i> (B3LYP-D3)	-4443.499207	-4443.481325	-4443.496808	-4433.454586

Table S2. Calculated relative energies (kcal mol⁻¹) of different spin states of [(TPFC)Mn^{III}(O₂)].

species	septet	quintet	triplet	singlet
$\Delta E(\text{BP86}/\text{def2-SVP})$	0.0	-1.4	-9.5	-4.1
$\Delta E(\text{BP86}/\text{def2-TZVP})$	0.0	-0.9	-9.0	-3.7
$\Delta H(\text{BP86-D3})$	0.0	-4.2	-12.8	-6.2
$\Delta G(\text{BP86-D3})$	0.0	-1.7	-8.8	-1.3
$\Delta E(\text{TPSSh}/\text{def2-SVP})$	0.0	7.7	1.2	19.7
$\Delta E(\text{TPSSh}/\text{def2-TZVP})$	0.0	8.6	2.7	20.7
$\Delta H(\text{TPSSh-D3})$	0.0	2.2	-3.6	13.6
$\Delta G(\text{TPSSh-D3})$	0.0	4.3	-0.3	18.0
$\Delta E(\text{B3LYP}/\text{def2-SVP})$	0.0	11.4	1.8	24.3
$\Delta E(\text{B3LYP}/\text{def2-TZVP})$	0.0	12.8	2.7	26.3
$\Delta H(\text{B3LYP-D3})$	0.0	6.8	0.5	18.6
$\Delta G(\text{B3LYP-D3})$	0.0	8.8	3.8	23.1

Table S3. Mulliken spin density of [(TPFC)Mn^{III}(O₂)].

species	B3LYP				TPSSh				BP86			
	Mn	O1	O2	Corrole	Mn	O1	O2	Corrole	Mn	O1	O2	Corrole
septet	4.01	0.99	1.00	0.00	4.00	1.00	1.00	0.00	4.01	0.99	1.00	0.00
quintet	3.95	0.07	0.09	-0.10	3.79	0.15	0.27	-0.20	3.29	0.27	0.43	0.01
triplet	4.00	-0.96	-1.01	-0.03	3.87	-0.83	-0.97	-0.07	3.09	-0.45	-0.68	0.04
singlet	2.24	-0.54	-0.73	-0.96	2.05	-0.46	-0.67	-0.92	0.00	0.00	0.00	0.00

B. with the axial OH⁻ ligand.

Table S4. The calculated expectation values of $\langle S^2 \rangle$ and absolute energies (in Hartree) of [(TPFC)Mn^{III}(O₂)(OH)]⁻.

species	septet	quintet	triplet	singlet	
$\langle S^2 \rangle$	12.0317	6.0302	2.9232	2.0246	
<i>E</i> (BP86/def2-SVP)	-4506.265554	-4506.284522	-4506.290010	-4506.277316	
<i>E</i> (BP86/def2-TZVP)	-4510.252334	-4510.267136	-4510.273419	-4510.255656	
<i>E</i> (DKH2-BP86)	-4519.995485	-4520.012624	-4520.019129	-4520.001447	
ZPE(BP86/def2-SVP)	0.378839	0.38098	0.381112	0.381832	
<i>H</i> _{corr} (BP86/def2-SVP)	0.433050	0.433556	0.433552	0.433786	
<i>G</i> _{corr} (BP86/def2-SVP)	0.283059	0.291233	0.292448	0.295284	
<i>E</i> _{disp}	-0.111538	-0.112978	-0.113161	-0.113586	
<i>H</i> (BP86-D3)	-4519.673973	-4519.692046	-4519.698738	-4519.681247	
<i>G</i> (BP86-D3)	-4519.823964	-4519.834369	-4519.839842	-4519.819749	
$\langle S^2 \rangle$	12.0776	6.1167	4.0354	2.0291	
<i>E</i> (B3LYP/def2-SVP)	-4506.032813	-4506.022166	-4506.032824	-4506.022336	
<i>E</i> (B3LYP/def2-TZVP)	-4510.051641	-4510.038505	-4510.051796	-4510.034680	
<i>E</i> (DKH2-B3LYP)	-4519.752607	-4519.743077	-4519.752743	-4519.736052	
ZPE(B3LYP/def2-SVP)	0.391695	0.393882	0.391697	0.393152	
<i>H</i> _{corr} (B3LYP/def2-SVP)	0.444413	0.444727	0.444425	0.445193	
<i>G</i> _{corr} (B3LYP/def2-SVP)	0.297531	0.306421	0.297360	0.302878	
<i>E</i> _{disp}	-0.098108	-0.099729	-0.098093	-0.099527	
<i>H</i> (B3LYP-D3)	-4519.406302	-4519.398079	-4519.406411	-4519.390386	
<i>G</i> (B3LYP-D3)	-4519.553184	-4519.536385	-4519.553476	-4519.532701	
species	septet	quintet	O ₂ -bound triplet	unbound triplet	singlet
$\langle S^2 \rangle$	12.0376	6.0803	3.0788	3.9978	1.1658
<i>E</i> (TPSSh/def2-SVP)	-4506.156324	-4506.160884	-4506.165697	-4506.156644	-4506.151603
<i>E</i> (TPSSh/def2-TZVP)	-4510.127725	-4510.129186	-4510.133697	-4510.127603	-4510.107167
<i>E</i> (DKH2-TPSSh)	-4519.806638	-4519.811321	-4519.815774	-4519.806640	-4519.794813
ZPE(TPSSh/def2-SVP)	0.389669	0.391831	0.391775	0.389722	0.391006
<i>H</i> _{corr} (TPSSh/def2-SVP)	0.442835	0.443170	0.443108	0.442734	0.443423
<i>G</i> _{corr} (TPSSh/def2-SVP)	0.295091	0.303852	0.304475	0.297118	0.300777
<i>E</i> _{disp}	-0.080753	-0.082806	-0.082822	-0.081523	-0.083424
<i>H</i> (TPSSh-D3)	-4519.444556	-4519.450957	-4519.455488	-4519.445429	-4519.434814
<i>G</i> (TPSSh-D3)	-4519.592300	-4519.590275	-4519.594121	-4519.591045	-4519.577460

Table S5. Relative energies (kcal mol⁻¹) of [(TPFC)Mn^{III}(O₂)(OH)]⁻.

species	septet	quintet	triplet	singlet
$\Delta E(\text{BP86}/\text{def2-SVP})$	15.4	3.4	0.0	8.0
$\Delta E(\text{BP86}/\text{def2-TZVP})$	13.2	3.9	0.0	11.2
$\Delta(E+\text{ZPE})(\text{BP86})$	11.8	3.9	0.0	11.6
$\Delta H(\text{BP86-D3})$	15.5	4.2	0.0	11.0
$\Delta G(\text{BP86-D3})$	10.0	3.4	0.0	12.6
$\Delta E(\text{B3LYP}/\text{def2-SVP})$	0.0	6.7	0.0	6.6
$\Delta E(\text{B3LYP}/\text{def2-TZVP})$	0.1	8.3	0.0	10.7
$\Delta(E+\text{ZPE})(\text{B3LYP})$	0.1	9.7	0.0	11.7
$\Delta H(\text{B3LYP-D3})$	0.1	5.2	0.0	10.1
$\Delta G(\text{B3LYP-D3})$	0.2	10.7	0.0	13.0

species	septet	quintet	O ₂ -bound triplet	unbound triplet	singlet
$\Delta E(\text{TPSSh}/\text{def2-SVP})$	5.9	3.0	0.0	5.7	8.9
$\Delta E(\text{TPSSh}/\text{def2-TZVP})$	3.9	2.8	0.0	3.8	16.6
$\Delta(E+\text{ZPE})(\text{TPSSh})$	2.4	2.8	0.0	2.5	16.1
$\Delta H(\text{TPSSh-D3})$	6.9	2.8	0.0	6.3	13.0
$\Delta G(\text{TPSSh-D3})$	1.1	2.4	0.0	1.9	10.5

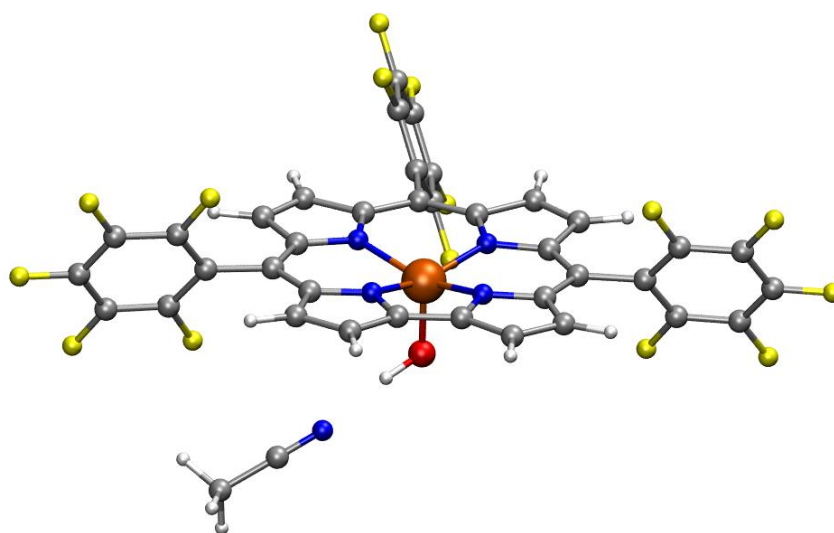
**Fig. S2** The TPSSh-optimized structure of [(TPFC)Mn(OH)(CH₃CN)]⁻.

Table S6. Mulliken spin density of [(TPFC)Mn^{III}(O₂)(OH)]⁻.

species	B3LYP				
	Mn	O1	O2	O(H)	Corrole
septet	4.01	0.99	1.00	0.19	0.00
quintet	3.17	0.29	0.53	0.08	-0.10
triplet	4.00	-0.96	-1.01	0.19	-0.03
singlet	2.24	-0.54	-0.73	0.05	-0.96
species	TPSSh				
	Mn	O1	O2	O(H)	Corrole
septet	3.81	1.00	1.00	0.20	0.00
quintet	3.08	0.30	0.54	0.10	-0.03
O ₂ -bound triplet	3.13	-0.52	-0.67	0.11	-0.05
unbound triplet	3.79	-0.99	-0.98	0.20	-0.02
singlet	1.95	-0.97	-0.98	0.07	-0.07
species	BP86				
	Mn	O1	O2	O(H)	Corrole
septet	3.68	0.97	0.97	0.25	0.13
quintet	2.71	0.46	0.64	0.14	0.06
triplet	2.89	-0.45	-0.60	0.15	0.02
singlet	1.12	-0.47	-0.63	0.04	-0.06

C. Binding energy of dioxygen to the Mn(III) corrole complexes.

Table S7. Absolute energies (in Hartree) for the key species of O₂ binding.

species	Mn ^{III} (quintet)	O ₂ (triplet)	Mn ^{III} -OH
<i>E</i> (BP86/def2-SVP)	-4280.144966	-150.2161514	-4356.048247
<i>E</i> (BP86/def2-TZVP)	-4283.848011	-150.3992109	-4359.853734
<i>E</i> (DKH2-BP86)	-4293.428953	-150.497184	-4369.483063
ZPE(BP86/def2-SVP)	0.364051	0.003632	0.375030
<i>H</i> _{corr} (BP86/def2-SVP)	0.411381	0.006940	0.424895
<i>G</i> _{corr} (BP86/def2-SVP)	0.280821	-0.016350	0.289084
<i>E</i> _{disp}	-0.09881996	-0.00000114	-0.10539793
<i>H</i> (BP86-D3)	-4293.116392	-150.490245	-4369.163566
<i>G</i> (BP86-D3)	-4293.246952	-150.513535	-4369.299377
<i>E</i> (TPSSh/def2-SVP)	-4280.054474	-150.2077112	-4355.94636
<i>E</i> (TPSSh/def2-TZVP)	-4283.742782	-150.3909299	-4359.736002
<i>E</i> (DKH2-TPSSh)	-4293.232878	-150.4964784	-4369.309891
ZPE(TPSSh/def2-SVP)	0.374276	0.003812	0.385399
<i>H</i> _{corr} (TPSSh/def2-SVP)	0.420547	0.007119	0.434300
<i>G</i> _{corr} (TPSSh/def2-SVP)	0.292365	-0.016149	0.300317
<i>E</i> _{disp}	-0.0720935	-0.00000072	-0.07700999
<i>H</i> (TPSSh-D3)	-4292.903053	-150.486770	-4368.952601
<i>G</i> (TPSSh-D3)	-4293.031235	-150.510038	-4369.086584
<i>E</i> (B3LYP/def2-SVP)	-4279.930220	-150.2049982	-4355.825639
<i>E</i> (B3LYP/def2-TZVP)	-4283.661573	-150.3898699	-4359.661795
<i>E</i> (DKH2-B3LYP)	-4293.202163	-150.4973652	-4369.249955
ZPE(B3LYP/def2-SVP)	0.376170	0.003869	0.387318
<i>H</i> _{corr} (B3LYP /def2-SVP)	0.421939	0.007176	0.435829
<i>G</i> _{corr} (B3LYP/def2-SVP)	0.294835	-0.016086	0.302071
<i>E</i> _{disp}	-0.08750655	-0.00000096	-0.09311206
<i>H</i> (B3LYP-D3)	-4292.867731	-150.490190	-4368.907238
<i>G</i> (B3LYP-D3)	-4292.994835	-150.513452	-4369.040996

Part II. Reaction of $[(\text{TPFC})\text{Mn}(\text{OH})(\text{O}_2)]^-$ with THF

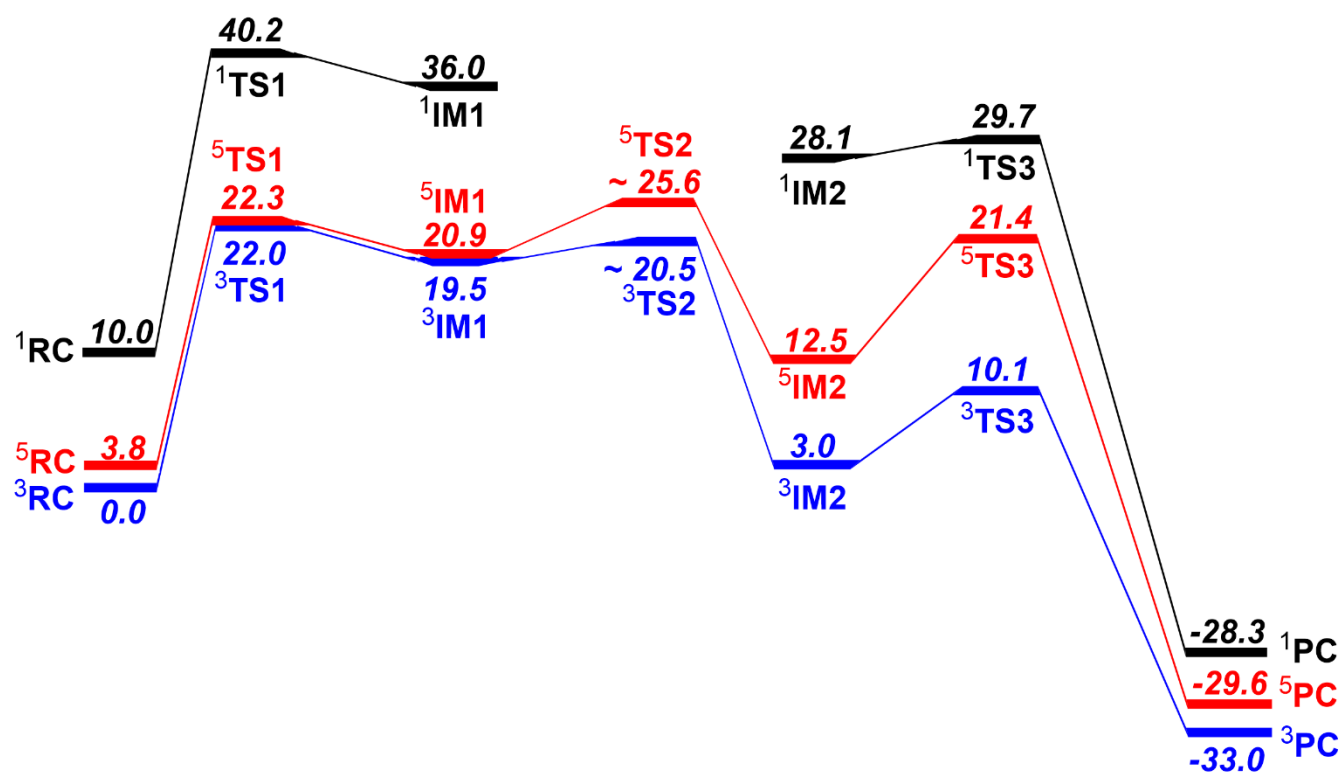


Fig. S3. Energy profile for the reaction of $[(\text{TPFC})\text{Mn}(\text{OH})(\text{O}_2)]^-$ with THF. Relative free energies (kcal mol⁻¹) were given at the TPSSh-D3 level.

Table S8. Absolute energies (in Hartree) of the key species involved in the reaction of [(TPFC)Mn(OH)(O₂)]⁻ with THF at the TPSSh level.

species	$\langle S^2 \rangle$	$E(\text{def2-SVP})$	$E(\text{def2-TZVP})$	$E(\text{DKH})$	E_{corr}	E_{disp}	G
³ RC	3.0653	-4738.471296	-4742.690887	-4752.485863	0.409097	-0.096424	-4752.173189
³ TS1	2.9923	-4738.432267	-4742.652374	-4752.446463	0.408713	-0.100453	-4752.138203
³ IM1	3.0412	-4738.436935	-4742.658652	-4752.452911	0.410763	-0.099899	-4752.142047
³ IM2	2.0148	-4738.477273	-4742.691502	-4752.487302	0.419097	-0.100170	-4752.168375
³ TS3	2.0469	-4738.459030	-4742.673709	-4752.473531	0.416698	-0.100218	-4752.157051
³ PC	2.7694	-4738.527174	-4742.749747	-4752.543029	0.413236	-0.095970	-4752.225763
⁵ RC	6.0700	-4738.467293	-4742.686605	-4752.480446	0.407957	-0.094620	-4752.167109
⁵ TS1	6.0541	-4738.430235	-4742.650311	-4752.444785	0.407374	-0.100225	-4752.137636
⁵ IM1	6.0419	-4738.436730	-4742.658488	-4752.450750	0.410224	-0.099317	-4752.139843
⁵ M2	6.0447	-4738.463890	-4742.674649	-4752.467751	0.415992	-0.101498	-4752.153257
⁵ TS3	6.0611	-4738.437737	-4742.653838	-4752.451603	0.413502	-0.101039	-4752.139139
⁵ PC	6.0347	-4738.524045	-4742.751098	-4752.538029	0.414945	-0.097205	-4752.220289
¹ RC	2.0255	-4738.456674	-4742.673231	-4752.465142	0.404743	-0.096824	-4752.157223
¹ TS1	1.7305	-4738.409761	-4742.624851	-4752.417940	0.405337	-0.096593	-4752.109196
¹ IM1	1.7220	-4738.417463	-4742.635421	-4752.430804	0.410513	-0.095565	-4752.115856
¹ IM2	0.0000	-4738.43993	-4742.673231	-4752.447622	0.421070	-0.101907	-4752.128459
¹ TS3	0.0000	-4738.437871	-4742.65272	-4752.445865	0.421825	-0.101828	-4752.125868
¹ PC	0.0000	-4738.523724	-4742.740903	-4752.539860	0.418498	-0.096879	-4752.218241

Table S9. Calculated relative energies (kcal mol⁻¹) for the key species involved in the reaction of [(TPFC)Mn(OH)(O₂)]⁻ with THF at the TPSSh level.

species	ΔE (def2-SVP)	ΔE (def2-TZVP)	$\Delta(\text{DKH})$	ΔG
³ RC	0.0	0.0	0.0	0.0
³ TS1	24.5	24.2	24.7	21.9
³ IM1	21.6	20.2	20.7	19.5
³ IM2	-3.8	-0.4	-0.9	3.0
³ TS3	7.7	10.8	7.7	10.1
³ PC	-35.1	-36.9	-35.9	-33.0
⁵ RC	2.5	2.7	3.4	3.8
⁵ TS1	25.8	25.5	25.8	22.3
⁵ IM1	21.7	20.3	22.0	20.9
⁵ IM2	4.7	10.2	11.4	12.5
⁵ TS3	21.1	23.3	21.5	21.4
⁵ PC	-33.1	-37.8	-32.7	-29.6
¹ RC	9.2	11.1	13.0	10.0
¹ TS1	38.6	41.4	42.6	40.2
¹ IM1	33.8	34.8	34.5	36.0
¹ IM2	19.7	11.1	24.0	28.1
¹ TS3	21.0	24.0	25.1	29.7
¹ PC	-32.9	-31.4	-33.9	-28.3

Table S10. Spin density distribution for the key species involved in the reaction of [(TPFC)Mn(OH)(O₂)]⁻ with THF at the TPSSh level.

species	Mn	O1	O2	O(H)	THF	Corrole
³ RC	3.11	-0.51	-0.51	0.11	0.00	-0.20
³ TS1	2.94	-0.04	-0.24	0.09	-0.67	-0.07
³ IM1	2.98	0.02	-0.05	0.07	-0.94	-0.07
³ IM2	1.94	0.03	0.01	0.08	0.00	-0.06
³ TS3	2.05	-0.04	-0.02	0.07	0.00	-0.06
³ PC	2.52	0.18	0.00	-0.09	0.00	-0.61
⁵ RC	3.07	0.31	0.54	0.10	0.00	-0.02
⁵ TS1	2.99	0.07	0.28	0.08	0.65	-0.08
⁵ IM1	2.98	0.02	0.02	0.07	0.95	-0.03
⁵ IM2	3.79	-0.01	0.01	0.04	0.00	0.16
⁵ TS3	3.68	0.14	0.06	0.10	0.01	0.01
⁵ PC	2.59	0.49	0.01	0.10	0.00	0.81
¹ RC	1.95	-0.96	-0.97	0.07	0.00	-0.09
¹ TS1	1.54	-0.39	-0.43	0.04	-0.69	-0.06
¹ IM1	1.29	-0.27	-0.15	0.05	-0.93	0.01
¹ IM2	0.00	0.00	0.00	0.00	0.00	0.00
¹ TS3	0.00	0.00	0.00	0.00	0.00	0.00
¹ PC	0.00	0.00	0.00	0.00	0.00	0.00

Part III. Mn(V)-Oxo Complexes with and without the Axial OH⁻ Ligand.

Table S11. Absolute energies (in Hartree) for [(TPFC)Mn^V(O)].

species	<i>E1</i>	<i>E2</i>	<i>E2+ZPE</i>	<i>G</i>	<i>H</i>
¹ Mn ^V (O)	-4355.168860	-4358.951122	-4358.571425	-4358.652367	-4358.524462
³ Mn ^V (O)	-4355.148294	-4358.932107	-4358.554347	-4358.636827	-4358.506901
⁵ Mn ^V (O)	-4355.145410	-4358.928846	-4358.552352	-4358.635786	-4358.504762

Table S12. Calculated relative energies (kcal mol⁻¹) for [(TPFC)Mn^V(O)].

species	$\Delta E1$	$\Delta E2(TZVP)$	$\Delta(E2+ZPE)$	ΔG	ΔH
¹ Mn ^V (O)	0.0	0.0	0.0	0.0	0.0
³ Mn ^V (O)	12.9	11.9	10.7	9.8	11.0
⁵ Mn ^V (O)	14.7	14.0	12.0	10.4	12.4

Table S13. Spin density distribution for [(TPFC)Mn^V(O)].

species	Mn	O	Corrole
¹ Mn ^V (O)	0.00	0.00	0.00
³ Mn ^V (O)	2.15	-0.01	-0.14
⁵ Mn ^V (O)	2.55	0.51	0.94

Table S14. Absolute energies (in Hartree) for [(TPFC)Mn^V(O)(OH)]⁻

species	<i>E1</i>	<i>E2(TZVP)</i>	<i>E2+ZPE</i>	<i>G</i>	<i>H</i>
[¹ Mn ^V (O)(OH)] ⁻	-4431.039474	-4434.915803	-4434.52503	-4434.607781	-4434.476035
[³ Mn ^V (O)(OH)] ⁻	-4431.037788	-4434.918989	-4434.530173	-4434.614865	-4434.480583
[⁵ Mn ^V (O)(OH)] ⁻	-4431.031849	-4434.914026	-4434.525013	-4434.609727	-4434.475545

Table S15. Calculated relative energies (kcal mol⁻¹) for [(TPFC)Mn^V(O)(OH)]⁻

species	$\Delta E1$	$\Delta E2(TZVP)$	$\Delta(E2+ZPE)$	ΔG	ΔH
[¹ Mn ^V (O)(OH)] ⁻	-1.1	2.0	3.2	4.4	2.9
[³ Mn ^V (O)(OH)] ⁻	0.0	0.0	0.0	0.0	0.0
[⁵ Mn ^V (O)(OH)] ⁻	3.7	3.1	3.2	3.2	3.2

Part IV. Bond Dissociation Free Energies and Reaction Energies

Table S16. Calculated bond dissociation energies of corresponding species.

species	<i>E</i> (def2-SVP)	<i>E</i> (def2-TZVP)	<i>G</i>
H	-0.499275101	-0.499871126	-0.510525126
THF-H(radical)	-231.6470925	-231.9018587	-231.8273917
THF	-232.3010329	-232.5568499	-232.4687359
BDE(C-H) (kcal mol ⁻¹)	97.1	97.3	82.1

species	<i>E</i> (def2-SVP)	<i>E</i> (def2-TZVP)	<i>G</i>
[(TPFC)Mn(O ₂)(OH)] ⁻	-4506.165702	-4510.133697	-4509.912044
[(TPFC)Mn(OOH)(OH)] ⁻	-4506.782641	-4510.754037	-4510.521651
BDE(O-H) (kcal mol ⁻¹)	73.8	75.6	62.1

Table S17. Calculated reaction energies.

species	<i>E</i> (def2-SVP)	<i>E</i> (def2-TZVP)	<i>G</i>	<i>H</i>
OH radical	-75.67095132	-75.76993585	-75.77857585	-75.75832685
[(TPFC)Mn(OOH)(OH)] ⁻	-4506.782641	-4510.754037	-4510.436389	-4510.298895
[(TPFC)Mn ^V (O)(OH)] ⁻	-4431.037788	-4434.918989	-4434.614865	-4434.480583
Δ<i>E</i>¹ (kcal mol ⁻¹)	46.4	40.9	27.0	37.6

species	<i>E</i> (def2-SVP)	<i>E</i> (def2-TZVP)	<i>G</i>	<i>H</i>
OH ⁻	-75.78977428	-75.93492373	-75.94320073	-75.92361073
[(TPFC)Mn(OOH)(OH)] ⁻	-4506.782641	-4510.754037	-4510.436389	-4510.298895
[(TPFC)Mn ^{VI} (O)(OH)]	-4430.866227	-4434.744981	-4434.440021	-4434.306179
Δ<i>E</i>² (kcal mol ⁻¹)	79.5	46.5	33.4	43.4

¹ Reaction energy for the homolytic O-O bond cleavage: [(TPFC)Mn(OH)(OOH)]⁻ → [(TPFC)Mn(OH)(O)]⁻ + HO•

² Reaction energy for the heterolytic O-O bond cleavage: [(TPFC)Mn(OH)(OOH)]⁻ → [(TPFC)Mn(OH)(O)] + HO⁻

Part V. Cartesian Coordinates for all the Species

A. [(TPFC)Mn^{III}(O₂)]

B3LYP-Optimized ¹[(TPFC)Mn^{III}(O₂)]

C	1.254166523984	-0.595289088178	5.636430325353
C	-0.084787522620	-0.995061711124	5.909040692257
C	-0.829148014590	-2.040871146874	5.260398579765
H	-0.466701778035	-2.685132887966	4.462528173218
C	-2.087908699859	-2.046567775282	5.819152991790
H	-2.917475984452	-2.695018517788	5.546202348638
C	-2.123467614632	-1.005438970101	6.811375195420
C	-3.265277761848	-0.620723836996	7.595672820741
C	-3.279583353365	0.491493850517	8.457444404136
C	-4.325877518842	1.096944418446	9.250211497529
H	-5.345927344012	0.731379767924	9.351970258015
C	-3.795342518300	2.234848883848	9.839930017925
H	-4.313402652300	2.937965756412	10.489480183444
C	-2.426337848128	2.312414108953	9.421229012001
C	-1.285387060199	3.193758872801	9.571731096859
C	-0.970495151969	4.454862086026	10.178463011491
H	-1.640456600702	5.068450199806	10.777863884594
C	0.339414931431	4.744988270752	9.829747829440
H	0.900085194686	5.637555127286	10.101482675819
C	0.821073602352	3.655782892941	9.007524402524
C	2.032805366136	3.456789225941	8.322787922757
C	2.271656098629	2.345761388711	7.439124846137
C	3.482583487490	2.084715304405	6.706756733553
H	4.394598523814	2.675715576546	6.749803806963
C	3.271359490552	0.952745037044	5.952218594962
H	3.983213178230	0.472881816960	5.284462097360
C	1.926873864709	0.513677266711	6.216588011216
C	2.007090396726	-1.401133358745	4.629534158903
C	2.390951124294	-2.722530173724	4.896449783550
C	3.093375709370	-3.488250822010	3.965224870452
C	3.422902600322	-2.934669363639	2.726658089810
C	3.050678570472	-1.622277415397	2.429932222343
C	2.352489016031	-0.873353138236	3.377951445404
C	3.112966853350	4.468122666678	8.497348068460
C	3.544310912897	5.275506766074	7.434536905809
C	4.543306498010	6.235667921283	7.595552296952
C	5.136780857917	6.409557740233	8.847386543285
C	4.728474628351	5.622705389812	9.925586378172
C	3.725288049756	4.669920563043	9.742933816007
C	-4.509061079355	-1.430641093091	7.459662800303
C	-4.556009874969	-2.765389824383	7.887748879231
C	-5.713356874428	-3.536078598001	7.776419336551
C	-6.864607945417	-2.973705974543	7.221643132935
C	-6.848966512688	-1.648502930126	6.783684144324
C	-5.681018686441	-0.894599326856	6.907460867847
F	2.095300931089	-3.278163635621	6.071893565425
F	3.452357431798	-4.737072538884	4.251059172996
F	4.089190449629	-3.655027859893	1.832660634912
F	3.357869124898	-1.096195382975	1.247110293580
F	2.003421864188	0.373559869176	3.059404635443
F	2.985866985931	5.148086159539	6.230232812999
F	4.924980052831	6.991444532106	6.569299415109
F	6.088010080856	7.320676483474	9.011321341353
F	5.297927938735	5.782638444249	11.117320763467
F	3.366656694965	3.930154666848	10.792627015533
F	-3.476576030898	-3.328931616403	8.431260202445
F	-5.728407096882	-4.796999406606	8.200529201059
F	-7.971355815277	-3.698165430369	7.110711060627
F	-7.942683084742	-1.113825718883	6.246839516241
F	-5.699443007825	0.363373032179	6.465239590068
N	1.357615532999	1.368322948840	7.132279970416

N	-0.197358308042	2.749444128026	8.898557035023
N	-2.156356817804	1.257524271380	8.616536919128
N	-0.894677803086	-0.390172412855	6.838972957840
Mn	-0.331079056965	1.021300446801	8.052243421265
O	0.355493402693	-0.009030496003	9.443447052213
O	-0.373002551446	-0.919819430220	9.928426268614

B3LYP-Optimized ³[(TPFC)Mn^{III}(O₂)]

C	1.219823285212	-0.525349609720	5.532741624030
C	-0.115211450964	-0.916338949578	5.802222259148
C	-0.831032478553	-2.032527268798	5.240691675126
H	-0.436665911055	-2.730235307939	4.505190189153
C	-2.091522721554	-2.042196678081	5.788838557784
H	-2.888386794516	-2.750108397722	5.570978224944
C	-2.189279879471	-0.934635925984	6.702482464266
C	-3.307498937273	-0.570186680295	7.488346366689
C	-3.319845285854	0.567031156895	8.339108763203
C	-4.304895736231	1.077638680852	9.251680793515
H	-5.285825654731	0.642865142058	9.435554722608
C	-3.775651424048	2.211074714133	9.866619842173
H	-4.261642744274	2.832501392588	10.616749485793
C	-2.467046432383	2.397861711701	9.339806475097
C	-1.340678044240	3.260418293765	9.499898703529
C	-0.959272107802	4.428000905909	10.219005545636
H	-1.580762873225	4.984177819013	10.918633560453
C	0.352503468080	4.722589382411	9.851758255857
H	0.949918544516	5.558890569338	10.210486321301
C	0.783678811713	3.727827075624	8.908821647148
C	2.011669457492	3.531923284922	8.223083144926
C	2.232104017897	2.461526020370	7.325387650998
C	3.459533424837	2.133028965367	6.650011564571
H	4.393967373478	2.682760434885	6.741242127392
C	3.244363006457	0.999587405095	5.902399450610
H	3.974218590481	0.478269232073	5.286847129641
C	1.874915959254	0.598774045559	6.095048337928
C	2.005956820200	-1.375072029742	4.589120243918
C	2.401823541522	-2.676483836449	4.928709094215
C	3.135259642317	-3.480543938631	4.055019755523
C	3.496327162193	-2.984521410465	2.801368269790
C	3.120202023799	-1.692048013125	2.432486869008
C	2.384161467759	-0.908435933191	3.322471628990
C	3.119234586750	4.498475868372	8.468509513626
C	3.586301126217	5.351860679151	7.458056726912
C	4.614172112909	6.269422508386	7.679223507912
C	5.202160928030	6.354842874662	8.942195914812
C	4.759868191222	5.521102532733	9.970405268120
C	3.731754190274	4.609730243865	9.725134439096
C	-4.529750434650	-1.420883794130	7.434982022883
C	-4.531912578537	-2.741285582988	7.908096090909
C	-5.675216063516	-3.540548630228	7.869245924343
C	-6.862879072844	-3.020818350795	7.352171966854
C	-6.896126318348	-1.709070728848	6.876665453206
C	-5.739686813331	-0.929376324941	6.923433785288
F	2.081671441213	-3.181984431847	6.121740878662
F	3.497523264480	-4.711697061565	4.411329294977
F	4.195833843036	-3.740577333392	1.961556486787
F	3.459274990716	-1.218180583780	1.234834463681
F	2.036538088048	0.319742851028	2.932438279825
F	3.040195952258	5.308943537164	6.241170719370
F	5.029810103563	7.068013288949	6.697999357716
F	6.180585958212	7.225977651415	9.164417052418
F	5.324622035548	5.594665506117	11.174101796031
F	3.344839486482	3.821074784014	10.729814923801

F -3.420061159021 -3.269195667437 8.423826833279
 F -5.642652862378 -4.789168313334 8.330953580639
 F -7.957816178316 -3.772527035997 7.312044563753
 F -8.025935703479 -1.212792907627 6.376165554385
 F -5.807632341053 0.315787859307 6.448026961477
 N 1.291091619871 1.504225976827 6.957538673420
 N -0.265961677482 2.873995009523 8.729135111819
 N -2.240018088277 1.397711613332 8.418756214198
 N -0.967092975630 -0.269253754731 6.674223283492
 Mn -0.523640391856 1.368298175726 7.577035797093
 O 0.211647199985 -0.273502888330 9.683726150922
 O -0.446352581130 -1.228973823442 9.991540663330

F 3.331434884712 3.821885619035 10.756068006702
 F -3.407268408937 -3.272154437328 8.457674142499
 F -5.624275380113 -4.800844725901 8.360518365059
 F -7.937564541126 -3.796755959081 7.325693493577
 F -8.010455309350 -1.241314203480 6.379097398035
 F -5.798442029915 0.295993860883 6.456507704303
 N 1.302312234448 1.480358882358 6.985159989210
 N -0.258286754536 2.862097973096 8.746327053443
 N -2.235376571682 1.393121846696 8.432805208890
 N -0.961199972878 -0.281698383335 6.689730859855
 Mn -0.478782909142 1.289051045736 7.683464682615
 O 0.171061152585 -0.153803215939 9.512260013054
 O -0.506062055368 -1.102458498658 9.843389791258

B3LYP-Optimized ⁵[(TPFC)Mn^{III}(O₂)]

C 1.220518207633 -0.533741282546 5.539720816696
 C -0.114621533694 -0.924559894973 5.809644134865
 C -0.834442272193 -2.036154410571 5.245142021036
 H -0.446087812821 -2.728223373325 4.501219759495
 C -2.090272503048 -2.050341275132 5.804483997172
 H -2.889725331347 -2.755225745369 5.586613422350
 C -2.180344655483 -0.947342659513 6.724347641868
 C -3.299612093943 -0.578760204310 7.511917026274
 C -3.319207986852 0.568036556850 8.347906405377
 C -4.317297039701 1.101276630168 9.234017732735
 H -5.304993221720 0.677684585283 9.406956137998
 C -3.791445008596 2.241970134836 9.837000620491
 H -4.287297222739 2.882017845097 10.564604240264
 C -2.471446884044 2.409959243906 9.330334685542
 C -1.341839548484 3.269880770091 9.491127309087
 C -0.968681477736 4.455657730442 10.185629160900
 H -1.600319274992 5.031963403264 10.859310625475
 C 0.347655069806 4.739540253245 9.828650317760
 H 0.940522455415 5.585730073087 10.171266968745
 C 0.789811503250 3.720388403364 8.916597668141
 C 2.021003524992 3.513602616727 8.242560671827
 C 2.243405933839 2.437622568139 7.349370175081
 C 3.466375362614 2.116737903806 6.662795028366
 H 4.399514243923 2.669471611902 6.747955170093
 C 3.246774840098 0.989956659279 5.906358502648
 H 3.971615120538 0.477147721050 5.277976934620
 C 1.880353719324 0.584591668909 6.108318616388
 C 2.001188389609 -1.375696013415 4.584538234559
 C 2.399676464884 -2.679320446004 4.911784070491
 C 3.129551745856 -3.474978186706 4.027496490019
 C 3.482655010070 -2.968130977494 2.77587245322
 C 3.102711571641 -1.673260014368 2.419276182355
 C 2.371103958683 -0.897650944828 3.319780968050
 C 3.127867166671 4.481040986220 8.487471835712
 C 3.603254049923 5.326684229457 7.474483186462
 C 4.628806487075 6.246203225282 7.698016719036
 C 5.205259380364 6.341439049160 8.965667430804
 C 4.754141562582 5.515519737893 9.996381422606
 C 3.728294988201 4.602221847266 9.749057805568
 C -4.520144554706 -1.431879175585 7.458344512312
 C -4.519007885579 -2.750709371034 7.935828710852
 C -5.659165189749 -3.554195456014 7.894346475958
 C -6.845974907001 -3.040804948097 7.368874779196
 C -6.881799859771 -1.731077153949 6.887959382062
 C -5.728802874085 -0.946540651013 6.937996703863
 F 2.086332829558 -3.194185146478 6.102358767865
 F 3.495466263331 -4.708274602398 4.371611098851
 F 4.178394880751 -3.716215506517 1.926212091027
 F 3.434279222545 -1.189419931279 1.223766487215
 F 2.019889884947 0.333328899209 2.942780832568
 F 3.067149395093 5.274596229996 6.253701973532
 F 5.052710785740 7.037636308689 6.714805863560
 F 6.181100207999 7.214594595855 9.189945414150
 F 5.307648572631 5.598802078866 11.204440809813

B3LYP-Optimized ⁷[(TPFC)Mn^{III}(O₂)]

C 1.248889995235 -0.521374599914 5.534763042245
 C -0.083008851826 -0.918622435317 5.814965947563
 C -0.806354650721 -2.024813368398 5.242038306632
 H -0.419521259480 -2.712810474659 4.493419183374
 C -2.064398589512 -2.036260616263 5.796242538608
 H -2.866397748856 -2.735985040791 5.570553601285
 C -2.152882813665 -0.939742696958 6.724749821877
 C -3.270686967306 -0.570952962091 7.509131179399
 C -3.280995757908 0.565230531059 8.362103172899
 C -4.278530166873 1.098284145903 9.248471447809
 H -5.268483725010 0.677971971598 9.417138810293
 C -3.750812714290 2.236899025821 9.855628232244
 H -4.247404597137 2.876658432052 10.583125309295
 C -2.430288023067 2.403851348251 9.351138437656
 C -1.307122897735 3.274341377796 9.498671050164
 C -0.935908457248 4.462932292365 10.188359195021
 H -1.563256002540 5.033163818253 10.871322577999
 C 0.374720540537 4.757941432235 9.816179155825
 H 0.964352521831 5.608780663195 10.153098227360
 C 0.814459685325 3.743481513976 8.898219890227
 C 2.041066295522 3.547203602519 8.208409693930
 C 2.263699905896 2.471319274652 7.317367433881
 C 3.484054028776 2.154887988056 6.622386042689
 H 4.413521298536 2.715653131851 6.695750972651
 C 3.268228868076 1.019518580001 5.877901081542
 H 3.992793970417 0.507650234270 5.248291179138
 C 1.905714729574 0.604302178894 6.093229641746
 C 2.025950145200 -1.359599887567 4.573494484190
 C 2.428915344433 -2.663420891609 4.895121900724
 C 3.155356572084 -3.456440208006 4.005591496932
 C 3.501830458253 -2.946740631802 2.753338834580
 C 3.117761536948 -1.651852932331 2.401618592875
 C 2.388804068597 -0.879604895540 3.307213112095
 C 3.141910752290 4.524580364634 8.440840743830
 C 3.601040083611 5.373447865344 7.423016847606
 C 4.621463993538 6.301399826273 7.635577175900
 C 5.209405331268 6.403033946571 8.897341657786
 C 4.774720461105 5.574566769765 9.932990983896
 C 3.754371454312 4.652393583729 9.696097343004
 C -4.497373076982 -1.414712535783 7.446185775394
 C -4.509091619775 -2.734728969102 7.920498193254
 C -5.655362070165 -3.529359410083 7.871675654090
 C -6.836130376137 -3.005453307525 7.343218025033
 C -6.859683408056 -1.694075744787 6.866234750519
 C -5.700507396147 -0.919085800744 6.922973642480
 F 2.123339564302 -3.182048206772 6.086438583217
 F 3.525205195004 -4.690039543651 4.345655244004
 F 4.195007054199 -3.692034253395 1.898613137196
 F 3.442377221865 -1.164920865472 1.205089373070
 F 2.032947020002 0.351047017755 2.932408202949
 F 3.053978646789 5.316688352898 6.207029667090
 F 5.029553003471 7.095261995227 6.647238071983
 F 6.180556662439 7.284454792004 9.111385219300

F 5.339364651433 5.663428185202 11.135814750534
 F 3.374911815861 3.869375621115 10.708102651698
 F -3.404251956108 -3.267748150220 8.445841357567
 F -5.632109375305 -4.777997910160 8.334323254277
 F -7.933709575082 -3.752981351162 7.293406756753
 F -7.982818451709 -1.193789630615 6.354463601576
 F -5.759124927749 0.325744487198 6.445064135983
 N 1.329294182165 1.501673089331 6.967745862650
 N -0.227487689392 2.876994594724 8.740777600530
 N -2.193423775675 1.383301133572 8.456572413759
 N -0.926579127454 -0.283658506118 6.702581354512
 Mn -0.458645287532 1.319585382225 7.654283426530
 O -0.472649908462 -0.986065867579 10.471220414521
 O -1.284967813989 -1.818030855900 10.173568532761

F 6.096709557384 7.313053403642 9.011645601133
 F 5.272929036845 5.804076493119 11.128724597294
 F 3.334533658553 3.954256320809 10.802213504858
 F -3.450641334937 -3.333655432293 8.419727786732
 F -5.700787034459 -4.812160570165 8.194550263343
 F -7.956739759375 -3.714551377807 7.125193017486
 F -7.945541021008 -1.123090263989 6.275659371284
 F -5.703647646870 0.364028533692 6.488365751946
 N 1.344170088220 1.378274213221 7.126932120597
 N -0.202452002240 2.751469801993 8.881331180823
 N -2.150075137030 1.263462328106 8.608494326316
 N -0.893834139485 -0.376043935076 6.840098374225
 Mn -0.336290869011 1.029836068903 8.044177794356
 O 0.303876581532 -0.003818876552 9.386855017971
 O -0.417445480929 -0.937703181838 9.860167115233

TPSSH-Optimized ¹[(TPFC)Mn^{III}(O₂)]

C 1.251067239462 -0.586508498402 5.634256162033
 C -0.088674220252 -0.984723746914 5.906836561445
 C -0.830242555521 -2.031269005833 5.260084568252
 H -0.465457314791 -2.672582147270 4.460715494162
 C -2.087240453326 -2.041626639105 5.824478623891
 H -2.917993512920 -2.691047370990 5.556717819371
 C -2.122051544762 -1.001446846058 6.815483043819
 C -3.260540126984 -0.619888838063 7.598198386869
 C -3.275536198936 0.495751231378 8.458628662290
 C -4.319120505758 1.094274310466 9.253032129680
 H -5.336090427299 0.721545010085 9.358983567871
 C -3.791248999052 2.236698907361 9.840110133587
 H -4.309198021299 2.938137625704 10.491011129434
 C -2.426932705529 2.320385855211 9.417019889278
 C -1.289963734807 3.199630059536 9.562437721510
 C -0.971952410610 4.456567406702 10.173534160818
 H -1.640702564595 5.067859174877 10.775924990772
 C 0.338294529739 4.744784298342 9.824827761489
 H 0.903340228760 5.633629722044 10.099516175529
 C 0.816941065516 3.658088240964 8.999576745081
 C 2.030515272245 3.460459348509 8.319518835162
 C 2.266857162323 2.348554450523 7.438208269173
 C 3.481767280494 2.080578008551 6.717876201139
 H 4.396118859037 2.667384199792 6.771784661274
 C 3.269932502034 0.948659329738 5.961943935129
 H 3.982873223113 0.459995970365 5.301489658437
 C 1.921593114310 0.519991724648 6.215390064347
 C 2.003052495999 -1.392904487399 4.630976476315
 C 2.361962269381 -2.724288680479 4.889225946693
 C 3.063912149047 -3.492454690938 3.958993478816
 C 3.417402507115 -2.931319788333 2.729450629007
 C 3.070597157825 -1.609356576744 2.440663607367
 C 2.373097230659 -0.858073362699 3.388082916186
 C 3.111714747157 4.466645956596 8.495679204504
 C 3.561087238820 5.259207673725 7.427633820225
 C 4.563378206118 6.216603616796 7.588944569020
 C 5.141707080120 6.403284753963 8.846947438855
 C 4.715953022022 5.631940780000 9.930725159508
 C 3.709729479455 4.681827415739 9.747263179575
 C -4.499826734055 -1.433002784896 7.465647301916
 C -4.537712948317 -2.771913527823 7.885084941953
 C -5.693099787692 -3.547025090631 7.777169431344
 C -6.850858824061 -2.985053431669 7.233562249712
 C -6.844554781144 -1.656169317971 6.803658644579
 C -5.678754889164 -0.897752292163 6.924974955171
 F 2.044153061419 -3.285544134490 6.058352757360
 F 3.401057645193 -4.751004043504 4.237065579008
 F 4.083746299415 -3.654713752104 1.835255772151
 F 3.400294112841 -1.077117783969 1.264636490880
 F 2.045181220839 0.398400441395 3.076854444813
 F 3.013584426164 5.120818143782 6.217340448773
 F 4.961675937064 6.959745655890 6.557397380830

TPSSH-Optimized ³[(TPFC)Mn^{III}(O₂)]

C 1.226375424782 -0.545766017733 5.562027958633
 C -0.108997769097 -0.934815621615 5.830358175613
 C -0.834771766599 -2.030133721023 5.247323988544
 H -0.449799494163 -2.708283612451 4.488744908721
 C -2.090957789611 -2.046156885690 5.809507651112
 H -2.899046572283 -2.737940692399 5.581047799622
 C -2.171115345891 -0.958422308679 6.745058311323
 C -3.292348711251 -0.586731129550 7.528133096672
 C -3.310181633261 0.562082478764 8.359055003886
 C -4.318741066217 1.113968275677 9.219402800665
 H -5.313009578106 0.700079395999 9.377193001181
 C -3.795579446962 2.259383926530 9.815270593852
 H -4.299234415227 2.915841202349 10.522013328470
 C -2.465727981631 2.409286226268 9.331439230575
 C -1.337623733073 3.266287116799 9.493501578644
 C -0.975071876031 4.470291593023 10.159802942712
 H -1.617164516778 5.063429813006 10.807872547604
 C 0.344328041656 4.747384287259 9.809224221272
 H 0.932425643442 5.605045450521 10.130835381217
 C 0.797682226537 3.706066477089 8.930333059582
 C 2.031105682334 3.496747002158 8.263578861747
 C 2.255681198706 2.413794657636 7.379662873335
 C 3.474519832501 2.098401607226 6.687134994268
 H 4.404727574661 2.656879550444 6.768008040528
 C 3.252343289722 0.972419393332 5.927933053558
 H 3.971247434574 0.461807596644 5.290750338984
 C 1.889813596647 0.565339526884 6.137989338070
 C 1.998172049162 -1.375365171519 4.592462427357
 C 2.379911017019 -2.691458693490 4.892619723538
 C 3.100735236442 -3.477785961903 3.991819754226
 C 3.460921490318 -2.948236788404 2.750663782077
 C 3.097947240211 -1.640579943899 2.420606173674
 C 2.374938821791 -0.874956992390 3.337255578443
 C 3.131482358288 4.470933164561 8.495864576969
 C 3.616708171071 5.293980659082 7.467515601900
 C 4.637454589720 6.222109414108 7.680523417245
 C 5.197662138713 6.350698839668 8.953430633032
 C 4.736296626540 5.549008788816 9.999826328073
 C 3.716066053817 4.626111125061 9.762366727054
 C -4.511976113612 -1.436540689629 7.466692890020
 C -4.508569909965 -2.761113878908 7.931318996324
 C -5.648079539557 -3.566007763421 7.883354050938
 C -6.836469600563 -3.048073173064 7.363594446628
 C -6.874899242656 -1.733059483719 6.894863575314
 C -5.722204477998 -0.947511120762 6.951083591710
 F 2.059470103910 -3.226158233039 6.074685300041
 F 3.452613240579 -4.723977643680 4.310364681428
 F 4.148825141894 -3.687907456793 1.884511187067
 F 3.435994883430 -1.136128861660 1.233387322644
 F 2.035777447351 0.368925312837 2.985696644123
 F 3.091558362979 5.212400895340 6.241450283779

F 5.070814980261 6.992816058178 6.682535548319
 F 6.169445384300 7.233630047082 9.168050488134
 F 5.276102312403 5.664141645650 11.213536769418
 F 3.308892533198 3.866858334167 10.783877105854
 F -3.393830189416 -3.285035753380 8.449263486398
 F -5.611969918669 -4.818540690797 8.338887139650
 F -7.928772643256 -3.805947125716 7.314307644397
 F -8.006100920026 -1.239992301769 6.389952801704
 F -5.791941369528 0.300528147981 6.478465607532
 N 1.311954952753 1.454194473546 7.025716182816
 N -0.244491123004 2.835086179346 8.771189765520
 N -2.215669383196 1.376569059076 8.452144786063
 N -0.947993489932 -0.298114479382 6.724864163543
 Mn -0.439818238123 1.223525402175 7.772730207284
 O 0.163082342602 -0.130369560966 9.489215978925
 O -0.531321568634 -1.072845366853 9.819409550449

F 3.126706354022 5.194307273055 6.256154097312
 F 5.116311335799 6.959290688386 6.718360373023
 F 6.190905276444 7.189497215636 9.214889376931
 F 5.263225202962 5.628064387127 11.250668234352
 F 3.283030078525 3.849178965675 10.800395340568
 F -3.361081373544 -3.273329399377 8.479467921655
 F -5.565173728374 -4.828820731636 8.390574002024
 F -7.893658553443 -3.848044792257 7.362658534462
 F -7.998248879728 -1.292232221909 6.414231548841
 F -5.799354917042 0.270528524273 6.482921467920
 N 1.309954192430 1.445758398408 7.034699640799
 N -0.253873827342 2.847460782481 8.746180194366
 N -2.225210778842 1.400749362638 8.418407100120
 N -0.947178913606 -0.295739372580 6.724516983601
 Mn -0.423569461901 1.186724692001 7.823779342220
 O 0.138700066949 -0.069463494004 9.482031395716
 O -0.602513640700 -1.012010672792 9.801802509865

TPSSh-Optimized ⁵[(TPFC)Mn^{III}(O₂)]

C 1.223781378055 -0.546367663899 5.561281195633
 C -0.110761010463 -0.935742275948 5.830070613584
 C -0.834550200815 -2.034040885885 5.252134240329
 H -0.451243637429 -2.7112335292149 4.493033169043
 C -2.086748998710 -2.053366877747 5.823085028647
 H -2.894931191727 -2.746880643151 5.600794816994
 C -2.163204908161 -0.961702655067 6.753816755780
 C -3.288764913372 -0.584308607569 7.534123000112
 C -3.316826327838 0.579043049395 8.338895219536
 C -4.331116453525 1.140852359486 9.186885519505
 H -5.324451048226 0.726218324503 9.347768455432
 C -3.813088444182 2.295488081635 9.766157598147
 H -4.319530559924 2.962336821987 10.460939728945
 C -2.480871461277 2.439536803280 9.283833430802
 C -1.349916952530 3.293712511743 9.449198198735
 C -0.989776210766 4.502765027213 10.109426922745
 H -1.638680913076 5.106962568292 10.740106724975
 C 0.335559406881 4.767213123572 9.776084671702
 H 0.925217632687 5.624305499531 10.096036503685
 C 0.793632111606 3.712865054308 8.915075447582
 C 2.031556881540 3.489395595555 8.268172934527
 C 2.257051656416 2.399612360200 7.389547207925
 C 3.476277783182 2.085019228858 6.698371342336
 H 4.406967693066 2.642101616037 6.781489172277
 C 3.251180482630 0.964355063716 5.932733975604
 H 3.967804964231 0.455129089745 5.292072573969
 C 1.888496055050 0.560458225976 6.142575822937
 C 1.992584256913 -1.368485788177 4.583059481718
 C 2.377370536473 -2.686073085994 4.871593875558
 C 3.094725443670 -3.463447566861 3.960331539512
 C 3.446007802738 -2.923307040331 2.721081505674
 C 3.078796701193 -1.613771280383 2.403012364686
 C 2.360874358556 -0.856274165146 3.330151334561
 C 3.137631269863 4.454553813198 8.510809388652
 C 3.640110883192 5.272668917121 7.487058329806
 C 4.666138540375 6.192195164610 7.711175408370
 C 5.214135256287 6.315260286289 8.990057306380
 C 4.735289299162 5.517563740579 10.031721399927
 C 3.708981544440 4.604220663822 9.783930908339
 C -4.500954862792 -1.444941487223 7.485033462849
 C -4.482475283499 -2.765471896743 7.960984711499
 C -5.614451677629 -3.581280520356 7.923854959017
 C -6.809007292844 -3.079442374033 7.402176900896
 C -6.861542267650 -1.769334402472 6.921125951430
 C -5.716808296558 -0.971715186227 6.967675180978
 F 2.063986619620 -3.229582007733 6.051094506150
 F 3.450726578051 -4.711063266873 4.266748503581
 F 4.129586170247 -3.654751930500 1.845236035899
 F 3.408421807246 -1.099714700224 1.218004943194
 F 2.017439367016 0.389745004913 2.991941666329

TPSSh-Optimized ⁷[(TPFC)Mn^{III}(O₂)]

C 1.249018211442 -0.523826346302 5.542438783739
 C -0.083330673516 -0.920708395328 5.820584328179
 C -0.807775053427 -2.019154965147 5.239306351874
 H -0.420512625408 -2.700798545001 4.484861451993
 C -2.067606764301 -2.030396552295 5.793584540644
 H -2.874172328848 -2.723709633482 5.563839799340
 C -2.151102347037 -0.941502715806 6.728522379815
 C -3.269320279290 -0.572655116038 7.513838394815
 C -3.277040828206 0.561608014834 8.368266608665
 C -4.273258761803 1.092253791899 9.255873327798
 H -5.262024757100 0.669208588877 9.424688580491
 C -3.746094528842 2.231195135972 9.863198493800
 H -4.241342552246 2.870604685637 10.591362384583
 C -2.426904629512 2.399146586251 9.357427120695
 C -1.305486724643 3.270279420409 9.502939601682
 C -0.936779164736 4.462393741069 10.186429788601
 H -1.565498738512 5.033696804217 10.866635992129
 C 0.372785619832 4.758701980824 9.810970385088
 H 0.961805592893 5.612533812410 10.141304700052
 C 0.813700225483 3.741024634261 8.898829280582
 C 2.039942984292 3.546138946538 8.209471681046
 C 2.264402301437 2.467248433107 7.321207001672
 C 3.485891561765 2.148200535648 6.633375908827
 H 4.415187435987 2.708844378271 6.711582879456
 C 3.270272350812 1.010088041642 5.889903953681
 H 3.994231736852 0.492456831854 5.264005831739
 C 1.907635454991 0.600369726784 6.101419321108
 C 2.023898559487 -1.360144453441 4.581351114670
 C 2.406543070111 -2.673584260628 4.892981241222
 C 3.131171858681 -3.467118327427 4.001598774814
 C 3.496391225837 -2.947814919226 2.757674565119
 C 3.133507933894 -1.643261744566 2.415752703970
 C 2.405594499837 -0.870980154862 3.322981374444
 C 3.138076496180 4.524508616296 8.435136650073
 C 3.609130326998 5.354487301473 7.405677265588
 C 4.629028567159 6.285359546078 7.611153995231
 C 5.203668717848 6.410183215967 8.877906022799
 C 4.757286436233 5.601556770912 9.925381523667
 C 3.738251685743 4.675534433338 9.694926405828
 C -4.496090395615 -1.411788260501 7.443502257209
 C -4.508112253201 -2.741952697910 7.892084411199
 C -5.656825046606 -3.533418948260 7.834966744778
 C -6.840149834061 -2.996117220669 7.323763444213
 C -6.864150576332 -1.674858554227 6.872154526824
 C -5.702303102303 -0.903586869921 6.936627328470
 F 2.083582673527 -3.199540014710 6.078644818151
 F 3.483112535027 -4.710513868295 4.332221581767
 F 4.188745103689 -3.694161329842 1.900288339994
 F 3.475912147685 -1.148178644746 1.225453497370

F 2.066221741139 0.369255099290 2.957784540647
 F 3.070870355168 5.277107621073 6.184751808593
 F 5.048241476470 7.062357691353 6.611581705314
 F 6.174932634159 7.295843552661 9.085626229878
 F 5.311358115820 5.712160860480 11.133409281846
 F 3.348200427275 3.908476119253 10.717685306301
 F -3.399946704993 -3.287140798860 8.402593208736
 F -5.634074171555 -4.792328750291 8.274683989825
 F -7.941219577501 -3.741311486869 7.266276994926
 F -7.990649215555 -1.162390069378 6.375122068411
 F -5.759525894879 0.351339701899 6.479919328405
 N 1.326551057335 1.499938832399 6.973438063670
 N -0.225805247812 2.867885704170 8.743998999382
 N -2.186075216423 1.378909467637 8.460521536569
 N -0.923684915871 -0.286474160969 6.714654502462
 Mn -0.455151694511 1.314235142913 7.660609189048
 O -0.436784845000 -0.981931286547 10.490477040618
 O -1.236753671444 -1.851688676154 10.262076745875

F 1.931087109911 0.377634145301 3.010523243973
 F 3.008404071580 5.183397502806 6.239611892189
 F 4.980650283789 7.013835412306 6.625235254222
 F 6.138576526223 7.288091695050 9.096107616902
 F 5.316781715519 5.709915090092 11.183246410520
 F 3.354450050021 3.867082369887 10.808376010255
 F -3.501712582159 -3.321008422519 8.494725483530
 F -5.767337045613 -4.810197097957 8.279477087794
 F -8.014447199300 -3.735353007897 7.131684312284
 F -7.980228047741 -1.159302655502 6.190732783342
 F -5.719616232859 0.334949640881 6.388364054867
 N 1.279119590643 1.381346706282 7.132678117167
 N -0.224840821288 2.734695041680 8.833402473549
 N -2.143095231230 1.271635744615 8.555114388246
 N -0.916281760127 -0.326006504143 6.842764255359
 Mn -0.294911916500 0.930760524246 8.187238799071
 O 0.257221807146 -0.028132506404 9.396676811066
 O 0.635904167682 -0.796799524276 10.310825628643

BP86-Optimized ¹[(TPFC)Mn^{III}(O₂)]

C 1.225174629642 -0.581585994539 5.613693440984
 C -0.104967177371 -0.960191036151 5.900338314951
 C -0.841591761284 -2.022046495479 5.265382177692
 H -0.460672748758 -2.671413495900 4.468658556510
 C -2.099959293907 -2.039322687963 5.832835582005
 H -2.936158740377 -2.699719805584 5.574635623366
 C -2.148328290104 -0.985144518250 6.814613694289
 C -3.293562292944 -0.625098189566 7.577533043325
 C -3.289698983154 0.503485321703 8.415314867645
 C -4.338430675048 1.115066909536 9.194359603327
 H -5.362073656860 0.734427646516 9.294224626512
 C -3.813227237448 2.268280255568 9.775075153521
 H -4.337724740025 2.987400731155 10.415914591902
 C -2.443032201144 2.349692465832 9.363143668534
 C -1.325938082955 3.211002411217 9.514764559403
 C -1.001555280828 4.467965295862 10.122872626887
 H -1.680710819201 5.091287868698 10.717090444440
 C 0.320835170429 4.747089176880 9.782120030145
 H 0.900187476008 5.636506743624 10.058446848036
 C 0.800037372918 3.656439618202 8.967521362773
 C 2.028136754402 3.461211309762 8.311988412073
 C 2.235276212637 2.352241810908 7.445550015502
 C 3.449176209553 2.074404707502 6.719599409821
 H 4.371508634365 2.663742805864 6.781696106142
 C 3.227308996956 0.948573755826 5.952564225341
 H 3.936514061107 0.448488111894 5.282886131492
 C 1.875478650562 0.522411334618 6.206320561506
 C 1.982663373088 -1.389870738643 4.609670868465
 C 2.396470069386 -2.707795612819 4.894603711218
 C 3.110617571874 -3.478359150107 3.961156106030
 C 3.422253230333 -2.929479040136 2.704377489669
 C 3.020345120641 -1.618855433920 2.390513246834
 C 2.309309361845 -0.866684821108 3.341231195042
 C 3.119603236205 4.458034174333 8.509223839903
 C 3.566237869045 5.284877222507 7.456090787511
 C 4.581840222451 6.238161359739 7.640965103874
 C 5.172878204726 6.383895427673 8.908838060770
 C 4.748125389942 5.576115917630 9.978618877126
 C 3.729810213710 4.630159951126 9.770249859656
 C -4.535487401874 -1.441997702077 7.453075823693
 C -4.584072090022 -2.772488607228 7.921286071105
 C -5.747618754020 -3.553411454588 7.818583305935
 C -6.901954340359 -3.002375027604 7.233835642535
 C -6.883969277670 -1.680075519344 6.755971991389
 C -5.708653854666 -0.917707381244 6.870132512634
 F 2.119090937407 -3.254527116717 6.088315844818
 F 3.498516931965 -4.724206480654 4.260718199674
 F 4.099989504501 -3.653131952061 1.808676604949
 F 3.311875808626 -1.099922226944 1.191307556068

BP86-Optimized ³[(TPFC)Mn^{III}(O₂)]

C 1.236382404563 -0.564594048902 5.580337627629
 C -0.101889139918 -0.948618681940 5.853164604643
 C -0.835351674623 -2.034547003014 5.250697457472
 H -0.452603623323 -2.699452726829 4.467519648502
 C -2.091386579769 -2.062762913565 5.830246054779
 H -2.913092636109 -2.748829776459 5.593007213739
 C -2.159247190446 -0.987131925124 6.787991352477
 C -3.291907743420 -0.615397464359 7.565248503874
 C -3.303906845523 0.544013416049 8.380545761852
 C -4.340294033773 1.141973018849 9.186916635520
 H -5.354357723062 0.744820216162 9.317395337025
 C -3.819608794295 2.305409340203 9.762496005171
 H -4.341295443679 3.004848276907 10.426837561263
 C -2.463706875264 2.415782945906 9.321765046269
 C -1.335741672716 3.269115679181 9.486342256562
 C -0.994867995758 4.512216749922 10.106085908179
 H -1.665274087813 5.139679543887 10.705708454993
 C 0.337318679939 4.777363571789 9.774806472857
 H 0.921790200891 5.659924960918 10.062669703488
 C 0.815232907702 3.689311662229 8.955259438530
 C 2.057837479002 3.477467329964 8.307649686794
 C 2.277017648163 2.378222438807 7.433635920079
 C 3.492150264232 2.077799002522 6.718246050834
 H 4.424627081490 2.650092332078 6.789067661003
 C 3.260985815015 0.955995318631 5.953380719112
 H 3.972447388440 0.453938868538 5.277245421275
 C 1.899936423052 0.539102292464 6.175025488805
 C 1.999751271875 -1.378627645200 4.584856197939
 C 2.412589703032 -2.696064941112 4.874597597199
 C 3.129777506925 -3.470446746617 3.946440713529
 C 3.449372974905 -2.925285339269 2.690165948734
 C 3.051147238165 -1.614801700368 2.371434375228
 C 2.334510924001 -0.860387130624 3.316185611115
 C 3.153637508398 4.464904899590 8.527072465125
 C 3.626358657787 5.290569555052 7.483974220305
 C 4.645935652244 6.235693377802 7.688615086967
 C 5.214040203168 6.376498959736 8.967306837447
 C 4.762917773835 5.571022249416 10.027993669298
 C 3.742611787621 4.632021950711 9.799138899935
 C -4.520332420080 -1.457791623970 7.490023971674
 C -4.532772159881 -2.783258053347 7.976146198311
 C -5.684807628716 -3.585729044527 7.916756263689
 C -6.865894521449 -3.062885020155 7.360762977982
 C -6.885543121682 -1.746392877014 6.867235994550
 C -5.720825203991 -0.962942966977 6.936353138608
 F 2.129593286359 -3.240627870598 6.068345494729
 F 3.514462402086 -4.716546179508 4.251057241766
 F 4.131129964001 -3.652268584028 1.799562045411

F 3.350366616954 -1.098748416375 1.172387504022
 F 1.960171168978 0.383924702873 2.979569929732
 F 3.090454384290 5.196989068546 6.256797302155
 F 5.069256419985 7.009517081835 6.681025497757
 F 6.182897324024 7.273599177937 9.173607283873
 F 5.310059078159 5.699476065346 11.243442839533
 F 3.343224736868 3.870236080363 10.829569350569
 F -3.426605907239 -3.307682667268 8.526073324795
 F -5.668149667937 -4.836936271858 8.393476837389
 F -7.967675413331 -3.816781680090 7.300279041598
 F -8.007228226268 -1.251937709039 6.328309581818
 F -5.769002036964 0.282887520215 6.438570994296
 N 1.320581968128 1.414389563445 7.092906064228
 N -0.221386831035 2.793586787345 8.811754964616
 N -2.186245205542 1.344106544741 8.486586910903
 N -0.933191057760 -0.316054181344 6.772632143884
 Mn -0.356894422311 1.058781071168 7.991322287260
 O 0.179888924826 -0.083734178723 9.386848617984
 O -0.529779885423 -1.055886199500 9.774830581321

F 3.390839783027 -1.117201684593 1.183313702491
 F 1.993433442486 0.378875700768 2.973143692064
 F 3.095443300807 5.205252335728 6.247699503815
 F 5.082635585817 7.005673594849 6.683663324073
 F 6.187952558731 7.257911136521 9.181087368608
 F 5.298523620619 5.683956768425 11.243849977785
 F 3.323421316725 3.866953549658 10.818712395098
 F -3.419508776462 -3.308911403857 8.493281663274
 F -5.657582212811 -4.843882506125 8.366750826943
 F -7.967900895932 -3.823111680838 7.297493258973
 F -8.022524257115 -1.251890456825 6.343856679716
 F -5.788287820301 0.289157607928 6.448455558268
 N 1.307360586327 1.436504821925 7.053537963721
 N -0.235409538285 2.807097145689 8.794579325308
 N -2.206023771459 1.357175620146 8.466591655771
 N -0.938757330643 -0.317259580244 6.759420735047
 Mn -0.382831156936 1.108941987109 7.923012244830
 O 0.345366826932 -0.034084994106 9.409736878751
 O -0.458170978455 -0.864639754998 9.936632939760

BP86-Optimized ⁵[(TPFC)Mn^{III}(O₂)]

C 1.230726507297 -0.561719659023 5.565839635879
 C -0.107598015412 -0.950299427201 5.840771346615
 C -0.841402636113 -2.036267877291 5.238016293230
 H -0.459615102187 -2.702527419360 4.455524320006
 C -2.099960936759 -2.059970439484 5.813062067830
 H -2.921813123402 -2.744931480112 5.573165181904
 C -2.167919265529 -0.983458888887 6.770112367778
 C -3.300196989669 -0.609842475651 7.548949956051
 C -3.316214706119 0.549055066416 8.368790087092
 C -4.344052383404 1.124601818114 9.202080705825
 H -5.352198609152 0.716960954766 9.345665744732
 C -3.820554611138 2.281264211358 9.790984182379
 H -4.334932025717 2.963082528893 10.478922036449
 C -2.473339657862 2.408374947690 9.327624607846
 C -1.342602542467 3.264810285881 9.494034281363
 C -0.995401142805 4.494569358580 10.133354492003
 H -1.657473593582 5.109880389239 10.754414828577
 C 0.334236317051 4.768960343362 9.789967028192
 H 0.919637448265 5.646702221039 10.090453276843
 C 0.804129546961 3.697928995071 8.945177408682
 C 2.044573517328 3.488256420274 8.289092016960
 C 2.265311426979 2.393288958877 7.407102615757
 C 3.487400277128 2.082193419927 6.707725058652
 H 4.423967049485 2.646334678500 6.789695416352
 C 3.259856332440 0.956342522192 5.936580891366
 H 3.979149190047 0.444430339344 5.286562110996
 C 1.893440896594 0.548459100169 6.152689583758
 C 1.998434070192 -1.382851430991 4.580148955836
 C 2.395900323817 -2.704095448692 4.875066404679
 C 3.116803709135 -3.485261892155 3.955644111222
 C 3.455809821376 -2.943743119028 2.702873609361
 C 3.073522183862 -1.629739666667 2.379129546091
 C 2.353153701068 -0.868220066735 3.315215225886
 C 3.144577099329 4.468820233150 8.516904013795
 C 3.626966441664 5.293323510938 7.477091934573
 C 4.650948801952 6.232197194508 7.687838948339
 C 5.214833964306 6.366945919518 8.969080223798
 C 4.754912298836 5.561833852117 10.026265153044
 C 3.729915262741 4.629451807820 9.791636715243
 C -4.526299798796 -1.455530081468 7.477286137614
 C -4.531065256701 -2.784490539285 7.954327422370
 C -5.681246150531 -3.589715301455 7.898444824889
 C -6.868017000637 -3.066417771243 7.355005111822
 C -6.895404477343 -1.746513653044 6.870941170413
 C -5.732783158397 -0.959832398952 6.937185540091
 F 2.095431337560 -3.245269929353 6.0660334938719
 F 3.487055506626 -4.734376002056 4.265433572244
 F 4.141015868610 -3.677416316769 1.820577202561

BP86-Optimized ⁷[(TPFC)Mn^{III}(O₂)]

C 1.221156810658 -0.559212494248 5.512243278448
 C -0.118632476002 -0.955418169420 5.787096620601
 C -0.846987463415 -2.050746000743 5.189994088627
 H -0.455486470852 -2.730186289274 4.423391854034
 C -2.116736940203 -2.064292661492 5.743258613149
 H -2.931602484828 -2.757321546142 5.501613566630
 C -2.199649842467 -0.980094183650 6.692194959663
 C -3.325895153631 -0.614367621985 7.480285579025
 C -3.327954941225 0.518484769192 8.346248363857
 C -4.331361527961 1.048697899317 9.237939613352
 H -5.329383961753 0.623107302724 9.401242227877
 C -3.799701844520 2.188791338770 9.858222262812
 H -4.299223219761 2.830670437183 10.594184222644
 C -2.472350506489 2.355185299457 9.355632856354
 C -1.346751735995 3.226594534851 9.509426738305
 C -0.977913339094 4.418682570841 10.205803739248
 H -1.612514253854 4.989330279620 10.894884985263
 C 0.339920875813 4.719108341087 9.831348939579
 H 0.934320091864 5.577059309261 10.169652892247
 C 0.782847789195 3.702351086631 8.907683589278
 C 2.016988715594 3.513721276328 8.218858078752
 C 2.241129166669 2.433785990675 7.320792154352
 C 3.468491555662 2.116463194470 6.631046991865
 H 4.405645394890 2.679755073245 6.715740104146
 C 3.250823167845 0.975623134277 5.876257492375
 H 3.980347261969 0.455346350086 5.244047836030
 C 1.881341879578 0.565438112176 6.084040877653
 C 1.998760324707 -1.392586571611 4.544468119768
 C 2.396887858529 -2.709223298770 4.860173838773
 C 3.127882435063 -3.503192071163 3.959728167364
 C 3.481738294016 -2.979111862237 2.703872425299
 C 3.101642483337 -1.670146054184 2.358651173872
 C 2.368128815893 -0.897626051379 3.275587906669
 C 3.118293699862 4.491520433467 8.456113756964
 C 3.582108328459 5.345721803631 7.431971921723
 C 4.609919644346 6.279362188900 7.649004186539
 C 5.198141250865 6.379530095201 8.922218603812
 C 4.758019650679 5.544659414172 9.964464849449
 C 3.730362699218 4.617022661292 9.722204016389
 C -4.560615806761 -1.447222473629 7.397046402858
 C -4.582942927336 -2.784842636014 7.848597914357
 C -5.742846029505 -3.575400976508 7.779389359606
 C -6.925370099563 -3.026887280743 7.252315843976
 C -6.937748843782 -1.696691981879 6.796957817124
 C -5.764394273192 -0.926936133510 6.873915710567
 F 2.086615183228 -3.236259678513 6.055860043508
 F 3.496213453176 -4.748207828704 4.291442246885

F 4.178603199305 -3.724412404021 1.839235131447
 F 3.432599138860 -1.173172909504 1.158969797581
 F 2.010457300679 0.343814997928 2.908644004179
 F 3.029582057809 5.291676448759 6.209215548699
 F 5.023155549400 7.080558431816 6.657776139090
 F 6.175376925846 7.265699019477 9.140886554778
 F 5.325322813794 5.632479337134 11.175082615872
 F 3.347276919479 3.823796148444 10.735949562892
 F -3.477545591552 -3.335332619039 8.376353765397
 F -5.733061619581 -4.839925980001 8.222209306507
 F -8.035536129685 -3.769114105101 7.183279283929
 F -8.061599242654 -1.176568284158 6.285454301665
 F -5.807681078365 0.333395435137 6.411961013997
 N 1.294623171092 1.465229230159 6.965968842927
 N -0.261408771774 2.825236440461 8.741720791736
 N -2.226868334089 1.333886480078 8.447422376331
 N -0.963574022366 -0.322773131158 6.691515725586
 Mn -0.489440254860 1.270889713396 7.650277592577
 O 0.708713001236 -0.538210204961 10.551454814326
 O 0.018940278499 -0.025095075899 11.412813998815

C -6.905646784975 -2.870351602034 7.997179096063
 C 3.526437656777 4.064765332385 7.308002285729
 C 4.464298337958 3.918196046937 8.340507876819
 C 3.790339768006 5.060360599300 6.355662251165
 C 5.605209821934 4.717455565562 8.428271037878
 C 4.926037760656 5.869043363759 6.419448122783
 C 5.836779714632 5.697997107748 7.462824551671
 F 6.921186811790 6.464554224056 7.535645325326
 F 6.477430608940 4.544348781825 9.420936656209
 F 4.290769967459 2.980744901805 9.275629070622
 F 5.140199343088 6.808633689755 5.498900399236
 F 2.936886381708 5.267281772289 5.349758917443
 F -5.557494086721 -0.435752682062 5.691651631508
 F -7.789151134548 -1.905262561119 6.031598059738
 F -8.010664565743 -3.591549265605 8.163483481335
 F -5.962402130256 -3.799963088306 9.952046999349
 F -3.716560838216 -2.354087864956 9.616583592007
 F 2.726666789625 -2.169249363378 4.321378478097
 F 3.512160404565 -3.521440960247 2.128441462832
 F 2.166594893142 -3.221334585781 -0.224901275274
 F 0.022408737549 -1.541177082359 -0.361739481740
 F -0.765519057850 -0.169074864460 1.818613868896
 O -1.537026511230 2.877582962944 5.679398271104
 H -0.899757670965 3.543825654921 5.386393296908

B. [(TPFC)Mn^{III}(OH)(O₂)⁻]

B3LYP-Optimized ¹[(TPFC)Mn^{III}(OH)(O₂)⁻]

C 0.508229235882 -0.356998180339 4.363281179252
 C -0.731258614534 -0.738744146195 4.942505283354
 C -1.568000082412 -1.848107346456 4.546097862827
 H -1.362611260523 -2.538068382923 3.730074077487
 C -2.636501816528 -1.886738906917 5.408237985363
 H -3.445828517647 -2.614478104337 5.410747137443
 C -2.478022447058 -0.806409753490 6.352933613074
 C -3.317556993995 -0.518920345881 7.457409706996
 C -3.016850342473 0.482476751799 8.420361246788
 C -3.651020957381 0.848347478262 9.661193814695
 H -4.561400672293 0.410143155661 10.067127868242
 C -2.874580601981 1.838722763214 10.255869174325
 H -3.057594751846 2.325552558732 11.212749647870
 C -1.775354161533 2.084786945631 9.377194215297
 C -0.580099150524 2.870336840102 9.334431048200
 C 0.115099101367 3.824973604840 10.138276978584
 H -0.214698205024 4.224755141141 11.096160299194
 C 1.295085226950 4.132965922957 9.466868639008
 H 2.069175354002 4.820941153839 9.803261331174
 C 1.323235212489 3.355053349845 8.254553955011
 C 2.302673885477 3.217184487494 7.233147359250
 C 2.180972840231 2.295362288569 6.164597459256
 C 3.161057738192 2.028398175785 5.138711434211
 H 4.126512655788 2.521590997231 5.042852324554
 C 2.663803274951 1.032974171602 4.333778577189
 C 3.152338301546 0.591251159048 3.467820039660
 C 1.368938598867 0.659422371795 4.854954360529
 N 1.109830175555 1.444664902373 5.950511718865
 N 0.173226653118 2.628322304692 8.217264390644
 N -1.911591723095 1.266311955514 8.288098280838
 N -1.313267886429 -0.133969935583 6.027326112145
 Mn -0.661110030336 1.553278596356 6.814466119909
 C 0.952584870732 -1.112019424446 3.154135901299
 C 2.048489527088 -1.986320884684 3.185302648234
 C 0.284458070625 -0.987041947733 1.927342961573
 C 2.467335941322 -2.696506538120 2.059002616694
 C 0.679872577054 -1.689945066056 0.788251740582
 C 1.778431293043 -2.547875920175 0.854615944123
 C -4.551354195103 -1.334497181633 7.642818713627
 C -4.702228410917 -2.211518333580 8.726938750858
 C -5.624184495497 -1.256830179779 6.742401667184
 C -5.857837264962 -2.971810532307 8.913084313696
 C -6.788064175395 -2.009598828860 6.905095636539

B3LYP-Optimized ³[(TPFC)Mn^{III}(OH)(O₂)⁻]

C 1.190239121308 -0.508165659651 5.470605855977
 C -0.144716958686 -0.906970966140 5.742943663264
 C -0.834139286759 -2.061272746245 5.212922132586
 H -0.422296246556 -2.779907593022 4.507382463719
 C -2.092837503107 -2.076734155516 5.760946590752
 H -2.874389666053 -2.810619529151 5.574210400705
 C -2.204198340970 -0.935252937330 6.638516194274
 C -3.324746456865 -0.574879030632 7.426326933712
 C -3.345512888916 0.572083981990 8.266643716806
 C -4.288193428487 1.010789585484 9.262941028512
 H -5.231930117876 0.524274082515 9.505341173030
 C -3.753951638843 2.137740374360 9.881911651038
 H -4.198442623311 2.708765953646 10.695854682491
 C -2.490121300071 2.386802055350 9.265448144734
 C -1.363545746953 3.254387842428 9.426137354083
 C -0.951649275147 4.346619358183 10.250532314417
 H -1.547203417621 4.834627375324 11.020807239211
 C 0.356433865119 4.652997896897 9.887563637510
 H 0.982899030349 5.430360460844 10.322136391281
 C 0.746385406725 3.735666028027 8.846827256767
 C 1.979725862748 3.533560798764 8.170142634470
 C 2.196473155732 2.471260131731 7.257958609781
 C 3.448879808853 2.114490691377 6.637241970756
 H 4.394395171665 2.632865684213 6.774295961322
 C 3.234530332239 0.980302058697 5.887675365874
 H 3.975803376449 0.427754815614 5.313781284976
 C 1.842247957020 0.623172404856 6.030153172051
 C 1.989654902179 -1.362798501343 4.543881647417
 C 2.379750583816 -2.665571442070 4.886803075605
 C 3.127033958045 -3.470704440842 4.025715643507
 C 3.513440359700 -2.974920848739 2.779881295375
 C 3.147199375122 -1.680950443857 2.407257860082
 C 2.395448674348 -0.897687059591 3.284349742337
 C 3.111345834981 4.457793613908 8.465145336946
 C 3.614656837881 5.333038475168 7.491174830146
 C 4.667229871455 6.211337519465 7.752717434800
 C 5.246754533739 6.234580650897 9.021975973074
 C 4.771018816283 5.377108369717 10.014750361310
 C 3.719260554877 4.505317208459 9.728168531483
 C -4.528471313410 -1.451815469860 7.412849852924
 C -4.495935977614 -2.769930369597 7.892826010321
 C -5.624522529887 -3.590941003278 7.890282079606

C -6.836795735018 -3.096710249116 7.407215614951
 C -6.907454731105 -1.787736799188 6.928783546198
 C -5.764425227228 -0.987111924308 6.937827809870
 F 2.044162228067 -3.173840315844 6.075491273181
 F 3.481909731517 -4.703370733695 4.388524759337
 F 4.227748244278 -3.732013941158 1.951536922509
 F 3.509597158780 -1.205755061927 1.215720829047
 F 2.057052747327 0.330753775503 2.884561898653
 F 3.079579128997 5.352022537320 6.268078537688
 F 5.115045930920 7.032527694457 6.803417298870
 F 6.249197038108 7.068552794630 9.283515701421
 F 5.328762466681 5.389097231094 11.225110864597
 F 3.307586501935 3.689452350965 10.701916465747
 F -3.363071098658 -3.277066030964 8.385502486596
 F -5.555180286942 -4.836968700715 8.358125068880
 F -7.919187130131 -3.869517533318 7.402287480922
 F -8.061392987703 -1.314131639604 6.459431846878
 F -5.872701589151 0.253467225360 6.456019262831
 N 1.249512661640 1.546051987276 6.854207015973
 N -0.324988791342 2.934659284555 8.595240760766
 N -2.299094326219 1.441828729672 8.292422908353
 N -1.002332312733 -0.250830896734 6.589727092941
 Mn -0.685547775186 1.602357843606 7.208223671256
 O 0.364929279481 0.026480835827 10.280768004131
 O -0.448960294491 0.283361352589 11.124564074695
 O -1.293868659152 2.623788562954 5.659045937298
 H -2.205830846176 2.384278399713 5.441919367379

B3LYP-Optimized ⁵[(TPFC)Mn^{III}(OH)(O₂)]-

C 1.226006601988 -0.557762770618 5.572457119180
 C -0.107898884924 -0.960665841081 5.847647705475
 C -0.826872724054 -2.069745658667 5.262189146745
 H -0.433226581041 -2.756745925841 4.515957539948
 C -2.088495993858 -2.080243215439 5.805151037993
 H -2.890269533239 -2.778755183305 5.574115020123
 C -2.177165439963 -0.982479465826 6.739236084618
 C -3.298951199509 -0.605545232877 7.515506653894
 C -3.306147953711 0.530942067384 8.370778872890
 C -4.293640714723 1.040527264436 9.285849510085
 H -5.274459026545 0.604676707157 9.469250062039
 C -3.764449784255 2.173472824416 9.900207199956
 H -4.248371365364 2.794676754310 10.652197480059
 C -2.454283186520 2.359847270121 9.368003833360
 C -1.330956241928 3.231407433552 9.520983959723
 C -0.957698333174 4.208519456038 10.239067108808
 H -1.581662670500 4.961338078294 10.939563350334
 C 0.350684965058 4.708065103742 9.869895603604
 H 0.946153670082 5.547975637870 10.224080435668
 C 0.782860250817 3.707440574827 8.926475848392
 C 2.013062990440 3.512603351834 8.238953947000
 C 2.239574327238 2.437808329026 7.345794868736
 C 3.469429817132 2.113911571536 6.664324304385
 H 4.401474793376 2.669467234362 6.747122234544
 C 3.254448362806 0.976076514857 5.924045492189
 H 3.982252678190 0.454845277070 5.305615148960
 C 1.883082112830 0.571818155313 6.129630416634
 C 2.006455348214 -1.394378548197 4.613511848412
 C 2.395035240649 -2.705136353719 4.926462658041
 C 3.122143693895 -3.498345206482 4.037564702856
 C 3.486419216267 -2.982620749377 2.793061837298
 C 3.118718762163 -1.681044981135 2.449321625277
 C 2.387645804398 -0.909558638207 3.353917721819
 C 3.114997384798 4.486280955532 8.478396170699
 C 3.585667570604 5.331637297884 7.462412989441
 C 4.608663498056 6.255876051226 7.679089340194
 C 5.188515236017 6.359340523912 8.944233401339
 C 4.743004031398 5.535223193355 9.978542245699
 C 3.721044042142 4.615954907226 9.736891650345

C -4.531280075245 -1.438469350327 7.445743929256
 C -4.552867414958 -2.767896693175 7.894091840726
 C -5.705579189549 -3.552702038353 7.838515954510
 C -6.886347382288 -3.009949873223 7.330027143078
 C -6.902042874231 -1.689289397409 6.879458538699
 C -5.735930604848 -0.925220887530 6.941608779803
 F 2.076525631557 -3.232072292534 6.111253755279
 F 3.477517507687 -4.738551637032 4.371801513151
 F 4.181106812775 -3.728174047081 1.938511721639
 F 3.459154974943 -1.187542954715 1.259073993082
 F 2.045554294225 0.326266323765 2.981538872518
 F 3.046314222744 5.277385895925 6.242415316591
 F 5.026283739785 7.046182241117 6.690987055488
 F 6.162279508140 7.237958093430 9.162638965878
 F 5.300753571261 5.624292501434 11.185289966003
 F 3.335902730204 3.835484576908 10.749218912645
 F -3.450754684678 -3.320949989134 8.405625860695
 F -5.688861003613 -4.810376495935 8.278238063752
 F -7.991035387161 -3.747880172601 7.274386333517
 F -8.025099263888 -1.170030923450 6.384917521732
 F -5.790242635829 0.327828794962 6.483812742939
 N 1.313024311617 1.474097860449 6.990697616527
 N -0.261026079402 2.855352448399 8.756241745068
 N -2.232626169797 1.361732240346 8.454254210791
 N -0.953602730939 -0.341937881201 6.729970784181
 Mn -0.528024560908 1.352332202615 7.573066825709
 O 0.268421496322 0.248966585547 9.147456689071
 O -0.456411003500 -0.644628382752 9.714112489844
 O -1.122438302677 2.355334912201 6.133242047876
 H -2.083206202999 2.254955574844 6.058508633190

B3LYP-Optimized ⁷[(TPFC)Mn^{III}(OH)(O₂)]-

C 1.215229079678 -0.475667696043 5.478330667892
 C -0.119179377397 -0.8736444814549 5.754250082899
 C -0.806829615832 -2.034489125916 5.236203092598
 H -0.394532605596 -2.758616164824 4.536576279767
 C -2.064007148631 -2.048223754659 5.787660376452
 H -2.844205307977 -2.785931174537 5.610370118721
 C -2.176060077742 -0.898778161215 6.654660744606
 C -3.294622324708 -0.536340647454 7.443537978334
 C -3.316748645610 0.615762629226 8.276247939604
 C -4.255055035688 1.053350190640 9.276944504751
 H -5.196210059462 0.564709385793 9.525031332451
 C -3.720143257470 2.182267022446 9.89184715597
 H -4.161191719174 2.752874825063 10.707953109688
 C -2.459973604660 2.432908836893 9.268966327591
 C -1.332276642332 3.299425277950 9.426465908995
 C -0.921023989194 4.398385673576 10.242054503206
 H -1.516501858719 4.891500238280 11.009131964424
 C 0.385893074457 4.704599240695 9.874592549768
 H 1.011422725910 5.486655684390 10.302039676864
 C 0.775803889570 3.780413020612 8.840063752710
 C 2.007478291881 3.577103554034 8.160695905534
 C 2.222644978029 2.511217255276 7.252384904735
 C 3.473700846763 2.150520142258 6.629626992559
 H 4.418970217242 2.673483356692 6.762226925258
 C 3.258613877214 1.016274414251 5.884994553122
 H 3.998885102549 0.462423972162 5.311072037671
 C 1.867169890622 0.658119943949 6.032576861355
 C 2.014483959774 -1.334876987807 4.555610527077
 C 2.408084668006 -2.634441470865 4.906496547476
 C 3.155281113238 -3.443754344364 4.049269331376
 C 3.538090495977 -2.95546717879 7.799370047948
 C 3.168318804156 -1.664813302098 2.418837627048
 C 2.416725723610 -0.877279972867 3.292239132788
 C 3.137891083679 4.505480800397 8.446905972982
 C 3.637006032018 5.375765114689 7.466315803225
 C 4.688035633563 6.258178538741 7.720046591645

C 5.270308395043 6.290755072901 8.987839676146
 C 4.798745974657 5.438480517174 9.987056071315
 C 3.748438527848 4.562440808076 9.708280560787
 C -4.491105935819 -1.423126996351 7.449490106303
 C -4.445188457281 -2.731708753710 7.954043230319
 C -5.567765638766 -3.560854785445 7.973150275016
 C -6.786466710203 -3.084913187486 7.487848568368
 C -6.869985626604 -1.785713738291 6.985512632068
 C -5.733069000551 -0.976471415308 6.973467104928
 F 2.075841934855 -3.135437751943 6.099203984338
 F 3.513445159429 -4.673248760779 4.419526476877
 F 4.252278133514 -3.716584555134 1.974618364285
 F 3.527388784273 -1.196778287452 1.223469816222
 F 2.075152285585 0.347873523272 2.885169048529
 F 3.099088801342 5.386023268173 6.244363877666
 F 5.131763702370 7.423126996351 6.764653068692
 F 6.271331167005 7.128731040598 9.241908721796
 F 5.359103584845 5.459398356065 11.196081805480
 F 3.340682127104 3.751852480936 10.688055106106
 F -3.306159294458 -3.221516502751 8.449203397401
 F -5.486526546640 -4.797495372261 8.463612604575
 F -7.862859827628 -3.865978597619 7.503370819689
 F -8.030234375807 -1.329516355163 6.514395187265
 F -5.853469527246 0.254743666182 6.470824284235
 N 1.275497006232 1.582902435712 6.855550991516
 N -0.293421234038 2.973585652089 8.597795708132
 N -2.272810533462 1.488194551229 8.294266849137
 N -0.976759161671 -0.211099002515 6.595960260195
 Mn -0.660123389490 1.644902682184 7.207298497040
 O -0.620995434924 -0.646786242899 10.389441041368
 O -1.463289805770 -1.494572435474 10.274440132891
 O -1.263262099804 2.670922061270 5.659253585933
 H -2.188487201682 2.466595557709 5.463464296666

C 3.105787351862 4.475412985194 8.461367879530
 C 3.604547585123 5.328003052917 7.463903264952
 C 4.652185109814 6.219787227156 7.701507611439
 C 5.231412496915 6.280611954251 8.970621195518
 C 4.760391325828 5.447189708983 9.986973621255
 C 3.713322209522 4.561608486103 9.723531612982
 C -4.511351846046 -1.419064164347 7.433186270700
 C -4.478716083362 -2.738140117355 7.912638314543
 C -5.605754156071 -3.562209696837 7.903104289493
 C -6.816762001412 -3.069514895498 7.412744138836
 C -6.887790717095 -1.759845699669 6.933989227812
 C -5.745899307210 -0.956523404494 6.950917829474
 F 2.027327739996 -3.173908016338 6.131208593761
 F 3.467639438998 -4.723548014518 4.457706329333
 F 4.239532907018 -3.764473014665 2.021327926784
 F 3.546622888861 -1.233147058619 1.270392186645
 F 2.090854640328 0.322256672350 2.926342546214
 F 3.066188553912 5.312929145670 6.239747972624
 F 5.095069636054 7.020438289045 6.729582176939
 F 6.230355825895 7.128754921874 9.209963430327
 F 5.319603519264 5.494557127999 11.198146176240
 F 3.306982382187 3.766794059830 10.719577979441
 F -3.345588436885 -3.242301869415 8.413199073613
 F -5.537205400319 -4.810063895434 8.372176008603
 F -7.899152031570 -3.845886308199 7.401051850397
 F -8.041674456506 -1.288268367275 6.456505490208
 F -5.853023917842 0.285844835125 6.467343902070
 N 1.246929921878 1.530576276012 6.906999639904
 N -0.302782926717 2.911082517630 8.658064626579
 N -2.269035444586 1.449531021621 8.343014071925
 N -0.984193917598 -0.217541546303 6.6197344665794
 Mn -0.643440909027 1.558065368774 7.332083701125
 O 0.169376041654 -0.139274741372 9.497965054957
 O -0.532070409440 -1.046010534035 9.87886906758
 O -1.269719876823 2.584870445075 5.989839528356
 H -2.240382101501 2.577026981109 6.054884280058

TPSSh-Optimized $^1[(\text{TPFC})\text{Mn}^{\text{III}}(\text{OH})(\text{O}_2)]^-$

C 1.201374997165 -0.506394192838 5.509571562825
 C -0.135835588002 -0.895096329543 5.774039692227
 C -0.829808397759 -2.042004599724 5.239811330917
 H -0.422766181894 -2.761116012874 4.531149727615
 C -2.090431949530 -2.044807971255 5.788190675590
 H -2.881402060707 -2.769249370274 5.601321000828
 C -2.187688371279 -0.901949266680 6.664000058002
 C -3.309373519099 -0.541582045222 7.456458069596
 C -3.336003451461 0.600501327141 8.298391102887
 C -4.302129672220 1.061315666175 9.261507766034
 H -5.263193754531 0.596201223705 9.477462217300
 C -3.767935944501 2.188976188879 9.880541236020
 H -4.227639228402 2.776191942705 10.674371509569
 C -2.483092584216 2.412002469330 9.296007550225
 C -1.350505362025 3.271975955241 9.461902456957
 C -0.953105372905 4.402077108058 10.243547290294
 H -1.558656151553 4.920736406162 10.985644037988
 C 0.355651817008 4.703580038140 9.877725325884
 H 0.971881971251 5.507582015907 10.277969985354
 C 0.755119922445 3.743322637220 8.879915152230
 C 1.979853810369 3.538233952859 8.194722849668
 C 2.195693881801 2.467861451228 7.287170863497
 C 3.446767819611 2.125036930288 6.657489065957
 H 4.386389397567 2.660499495698 6.784058634532
 C 3.238887794375 0.989230208020 5.909692945337
 H 3.978391639295 0.446920142852 5.322974018891
 C 1.854065071821 0.620852534747 6.070780257386
 C 1.999905405861 -1.367782309423 4.590477259002
 C 2.376180709864 -2.673305379838 4.940889914506
 C 3.124152757755 -3.487554069956 4.088052116470
 C 3.523985032168 -2.997935497192 2.843063651093
 C 3.171060178908 -1.701544067754 2.462767219398
 C 2.418873747718 -0.909194304126 3.332318280735

TPSSh-Optimized $^3[(\text{TPFC})\text{Mn}^{\text{III}}(\text{OH})(\text{O}_2)]^- (\text{O}_2\text{-bound state})$

C 1.221352528910 -0.551299771299 5.572010784890
 C -0.113751340518 -0.955455047488 5.842569573877
 C -0.829926374719 -2.064061895817 5.256662361845
 H -0.434105023745 -2.748289330945 4.508623852053
 C -2.091685520601 -2.078121737558 5.804122436112
 H -2.894691121630 -2.776602199408 5.576189082260
 C -2.178025785490 -0.982182627009 6.738374465770
 C -3.297739732472 -0.604718428182 7.519965368717
 C -3.304359693803 0.534335961016 8.370738197675
 C -4.293161888084 1.046143956843 9.282026050644
 H -5.273375874798 0.608527364540 9.465015033080
 C -3.766591791448 2.182614065930 9.892217004666
 H -4.251773024771 2.807004280134 10.640334243507
 C -2.455861496587 2.367890531881 9.361799986740
 C -1.333518505885 3.239137325215 9.514184875865
 C -0.962599117830 4.420904344682 10.226297448177
 H -1.589131003170 4.977215022293 10.921289777943
 C 0.346269343827 4.718145487846 9.858263307747
 H 0.942340185238 5.559910767059 10.207304442107
 C 0.780410956625 3.711108306524 8.922862371152
 C 2.012200039054 3.515160089225 8.239454463513
 C 2.241030199026 2.438659085238 7.346565998836
 C 3.471714794535 2.111574148843 6.671092786884
 H 4.404587702558 2.665368594216 6.759004448339
 C 3.254400444758 0.973394581465 5.928633652660
 H 3.980357073779 0.447338826401 5.311635472299
 C 1.882131220204 0.576176961977 6.130472468070
 C 2.001495222223 -1.386944437933 4.615305867923
 C 2.373630772094 -2.705176830692 4.921264549854
 C 3.101095570942 -3.499273815868 4.032593531255

C 3.482982308519 -2.976430424413 2.795411576595
 C 3.132800654028 -1.667322771130 2.458429164392
 C 2.400452444382 -0.895560954896 3.3625966833681
 C 3.114403932511 4.484495064481 8.480318938946
 C 3.605447146084 5.313336692979 7.458785513353
 C 4.631944402629 6.234216601736 7.676610761615
 C 5.194455693907 6.352155903006 8.949235391507
 C 4.728851462929 5.545521266450 9.989615680212
 C 3.704405198997 4.628755229713 9.746085891661
 C -4.525661870636 -1.440468047288 7.455149967211
 C -4.537379113852 -2.775370468769 7.890951858420
 C -5.687260480967 -3.565464519190 7.838278833752
 C -6.875771167945 -3.022530014680 7.345902201162
 C -6.902208349136 -1.696731224719 6.908401938224
 C -5.738386784319 -0.927960308303 6.966904753927
 F 2.039704393641 -3.237214910135 6.101834519733
 F 3.442053665163 -4.747369838256 4.360557161837
 F 4.179078192841 -3.723387794814 1.940107893986
 F 3.489849407482 -1.167860891313 1.273282137490
 F 2.071579741721 0.347893370369 2.996623910272
 F 3.079240402171 5.247219948381 6.231380274913
 F 5.068408699068 7.010187710650 6.682536939886
 F 6.172242228124 7.229015417193 9.169210786184
 F 5.272108286508 5.647642664311 11.204208242096
 F 3.301439511162 3.861297187702 10.764196497488
 F -3.426671431148 -3.327468342892 8.390222848655
 F -5.661424611419 -4.828852913043 8.267298980849
 F -7.979225095246 -3.766240841219 7.293213160903
 F -8.033787936528 -1.177892061041 6.427478481251
 F -5.801241577147 0.330319873931 6.518566034007
 N 1.310368775622 1.480250650008 6.991463581718
 N -0.261948558552 2.854358556905 8.753161721037
 N -2.227781650314 1.365637650504 8.450564782967
 N -0.959139065142 -0.335774845876 6.726629818352
 Mn -0.522493870959 1.342959772766 7.581342712353
 O 0.232351825180 0.246252576765 9.109304561954
 O -0.477388317461 -0.699490905076 9.598768719491
 O -1.112490936786 2.352933874621 6.139634979554
 H -2.078372313331 2.255660485449 6.083072193907

TPSSh-Optimized ³[(TPFC)Mn^{III}(OH)(O₂)]⁻ (unbound state)

C 1.193845369015 -0.501568498210 5.484785363778
 C -0.141558068073 -0.900188144430 5.755899603090
 C -0.833104633111 -2.046720297489 5.218104614552
 H -0.421921342940 -2.759114694363 4.505460659651
 C -2.092676844145 -2.062728593258 5.768795557059
 H -2.879400528958 -2.790519364258 5.578719199042
 C -2.197511642962 -0.929027944438 6.653807094136
 C -3.317726387246 -0.567704976087 7.443259175488
 C -3.335922384084 0.577869723188 8.283960213424
 C -4.285000850394 1.025805875387 9.268424418155
 H -5.233372614193 0.544164535248 9.502604455399
 C -3.752457652791 2.154758741251 9.885490616539
 H -4.202448713753 2.734461839968 10.689787637279
 C -2.481719109789 2.394237922777 9.280686203617
 C -1.357555801526 3.263011080301 9.437439086949
 C -0.952418424764 4.3711176657173 10.242783160355
 H -1.552404174991 4.869316603344 11.002611929212
 C 0.354280917608 4.678314769039 9.874980752644
 H 0.977218184228 5.466959830294 10.294192718841
 C 0.749687976961 3.746166305940 8.851133127301
 C 1.982194808651 3.545033423637 8.174012499968
 C 2.200435960105 2.478337420020 7.266031047618
 C 3.451666304139 2.119733460800 6.646670956031
 H 4.395635788453 2.644270676006 6.783817734664
 C 3.237269116243 0.985456648391 5.898656282679
 H 3.976494782562 0.429987107573 5.324461955089
 C 1.847114795857 0.629448639044 6.043183873708

C 1.991497787242 -1.355341586210 4.559726387459
 C 2.361583124890 -2.667214315817 4.894645081087
 C 3.108736329118 -3.473995825920 4.034173200286
 C 3.516106441563 -2.970340754566 2.797216264127
 C 3.170952908048 -1.667372306744 2.432446333428
 C 2.418216047933 -0.883037449303 3.308605465185
 C 3.110777076352 4.472395222464 8.458164547251
 C 3.626598918565 5.324320861735 7.468518517949
 C 4.679835052894 6.205713689693 7.719655055352
 C 5.247268299107 6.256496049515 8.994530891968
 C 4.759299718870 5.423375759674 10.003228601457
 C 3.707564759903 4.547596959470 9.726388400775
 C -4.520632704131 -1.441678858483 7.425673470442
 C -4.485615388743 -2.767233242574 7.887850124659
 C -5.614899964963 -3.588159009747 7.881852972183
 C -6.830839463961 -3.086072519805 7.413756118059
 C -6.904708436233 -1.769790899416 6.953574373988
 C -5.760615865671 -0.969786970673 6.965480691648
 F 2.007704114648 -3.181101116786 6.077818277268
 F 3.445895310900 -4.715802793147 4.389785621299
 F 4.231501253951 -3.729533633690 1.968640271796
 F 3.553028425661 -1.185646791070 1.247518523671
 F 2.096454475673 0.354403484205 2.916310728173
 F 3.099792364185 5.318184708549 6.239530727379
 F 5.139073992961 7.005857357546 6.755219656911
 F 6.251219555024 7.094612912014 9.246702641181
 F 5.307727738099 5.460716851217 11.219455358860
 F 3.285507218322 3.751531701615 10.714687255129
 F -3.348294612864 -3.280341802800 8.369311046961
 F -5.543618303483 -4.841861779278 8.334165260210
 F -7.915185339820 -3.859437518587 7.405775484529
 F -8.063187713331 -1.289324630808 6.497039081255
 F -5.870134570766 0.278675076004 6.498962087062
 N 1.251541408427 1.551743555188 6.869041693163
 N -0.315583990964 2.929837961022 8.611830851117
 N -2.280444785770 1.440036059035 8.315369297632
 N -0.994518144209 -0.245356293890 6.611219955427
 Mn -0.669125550972 1.588586293995 7.247449079149
 O 0.303001346874 -0.125836383310 10.107811201685
 O -0.619981025612 -0.243235164831 10.876023401221
 O -1.282851255670 2.599497696932 5.712821759809
 H -2.191037382151 2.332182700739 5.496478305540

TPSSh-Optimized ⁵[(TPFC)Mn^{III}(OH)(O₂)]⁻

C 1.220287911605 -0.548745355640 5.565578068343
 C -0.113986275252 -0.951369195621 5.838475536090
 C -0.829639208637 -2.061720277867 5.256460357353
 H -0.433597822126 -2.747920064014 4.510404693827
 C -2.090866501897 -2.074312273594 5.804527394995
 H -2.893972193630 -2.773573840047 5.579533413915
 C -2.177153871253 -0.975860459202 6.735234743300
 C -3.298111000962 -0.600001874302 7.514801099443
 C -3.307979304895 0.541326806702 8.361726630739
 C -4.292635545291 1.045652002620 9.281352838228
 H -5.268765070791 0.601901076662 9.471178509853
 C -3.767021037472 2.183274473384 9.890206312220
 H -4.248649734190 2.803050803644 10.644393514317
 C -2.461656351141 2.375896878052 9.349564929552
 C -1.338908445777 3.246175225599 9.502423484536
 C -0.964426751671 4.420829474869 10.222543876059
 H -1.589115174871 4.973860870204 10.921749369619
 C 0.345980240201 4.716557017426 9.856773253858
 H 0.944800524032 5.553679126008 10.212116279108
 C 0.776843350672 3.715532993905 8.914972031343
 C 2.009555210785 3.516610732619 8.234835775643
 C 2.236111817115 2.440482638534 7.342144905631
 C 3.467981459174 2.111213367542 6.671415765425
 H 4.401523083974 2.663100952586 6.763666048322

C 3.251515941223 0.973588403380 5.927988782260
H 3.978894716006 0.445538461949 5.314427850381
C 1.878447322535 0.578900811109 6.124272940104
C 2.001265810391 -1.385408664349 4.610722293075
C 2.372701328046 -2.703484227786 4.918276279751
C 3.101125283397 -3.498383855568 4.031127738264
C 3.484807392152 -2.976473159842 2.794094492057
C 3.135503991774 -1.667493092117 2.455686334970
C 2.402168721866 -0.894873540897 3.358305902444
C 3.115178647368 4.480883508241 8.480755870245
C 3.609564093829 5.312306499941 7.463034332194
C 4.639214571587 6.228557702085 7.685448419627
C 5.201561373630 6.338630168493 8.958861514665
C 4.732694999190 5.529006563796 9.995463529327
C 3.704985531126 4.617096906903 9.747431408331
C -4.522630829324 -1.440945155376 7.454904268820
C -4.528173883206 -2.774733549611 7.894284298650
C -5.675361555838 -3.569044857953 7.846894055166
C -6.867234639714 -3.031624067198 7.356560806485
C -6.899786700434 -1.707040357890 6.915784771577
C -5.738653637816 -0.933870981944 6.969179001552
F 2.037139605505 -3.234436814441 6.098820417849
F 3.441340745772 -4.746282113673 4.360407718465
F 4.181821778062 -3.724204629205 1.940277890802
F 3.494400499718 -1.168966885392 1.270749690635
F 2.074306913877 0.348512802914 2.991287756261
F 3.083976824600 5.252790192151 6.235082028638
F 5.079070575995 7.007239220640 6.695065530797
F 6.182374069638 7.210918259157 9.183191802570
F 5.275784974559 5.623770350053 11.210659304720
F 3.298435273243 3.846650015602 10.761777124166
F -3.414131147359 -3.321467097716 8.391857831250
F -5.643779172256 -4.831170377534 8.279090483020
F -7.968067453512 -3.779454718154 7.308916850170
F -8.034610735561 -1.193491346569 6.436962515511
F -5.807299236908 0.323140767558 6.518252927394
N 1.302871227354 1.483822909732 6.982891179822
N -0.269139047193 2.864350176874 8.736457248163
N -2.236740886217 1.379260957869 8.432361099740
N -0.957704749591 -0.328024131329 6.721989626793
Mn -0.533466972416 1.362906897290 7.559213436036
O 0.225888720826 0.273523630537 9.130342354072
O -0.508636442064 -0.650938426158 9.644245246006
O -1.128135560518 2.358578960200 6.120608201696
H -2.091833591041 2.245398784155 6.054115213763

TPSSh-Optimized ⁷[(TPFC)Mn^{III}(OH)(O₂)]-

C 1.206331454449 -0.473811619160 5.488447613681
C -0.128756256448 -0.871625110523 5.762065785005
C -0.817901412546 -2.024524825329 5.234594149604
H -0.405409628160 -2.742549266140 4.528380591725
C -2.076917091069 -2.038387041777 5.786377847195
H -2.862146918053 -2.769775109439 5.603939944644
C -2.183343290054 -0.896766562374 6.661133395123
C -3.303268240617 -0.532853713354 7.449605981474
C -3.323256643846 0.617980512575 8.282965549657
C -4.267642310938 1.063150914120 9.273095748839
H -5.212677194237 0.578184513428 9.513906837986
C -3.734279639194 2.193535295954 9.886963785537
H -4.180260211650 2.771436689316 10.694805113559
C -2.467975399158 2.436216198263 9.274140988328
C -1.342359327485 3.303747734719 9.429282662442
C -0.936462847918 4.413541024264 10.232030304000
H -1.536075190300 4.913868002575 10.990740404496
C 0.370123380573 4.719519353618 9.862816264986
H 0.993570312214 5.508790619036 10.280111140877
C 0.764615400059 3.784625423920 8.841225428179
C 1.996535103193 3.581441856738 8.163721782245

C 2.213624744630 2.512134804309 7.258334157804
C 3.465326888143 2.149667368185 6.642153377452
H 4.409903445741 2.673177267833 6.779129118346
C 3.250380887870 1.012935486686 5.898087735289
H 3.989681478783 0.453883498238 5.327453720493
C 1.859495617953 0.659560624295 6.042202490703
C 2.004906012364 -1.332281710939 4.568483483333
C 2.376801929941 -2.641661427938 4.911014563921
C 3.124964022890 -3.452481878939 4.055226451324
C 3.531800365766 -2.955468859577 2.815419188337
C 3.185044372247 -1.655052954130 2.443155794014
C 2.431291561583 -0.866637942998 3.314757345744
C 3.125752705664 4.508925819685 8.444743192496
C 3.642650150403 5.356709633801 7.452059301206
C 4.696464029107 6.238241360642 7.700220877086
C 5.263573060318 6.29342036553 8.8975051241134
C 4.774608780924 5.464502440165 9.986710774399
C 3.722330772786 4.588462146072 9.712822201594
C -4.501055598827 -1.413933826529 7.446189090098
C -4.456791600181 -2.733407052148 7.924997309769
C -5.581978861175 -3.560021993252 7.934160677302
C -6.802672607673 -3.070094559049 7.465586113297
C -6.885575403167 -1.760077068927 6.989432945636
C -5.745622168391 -0.954112971371 6.986367403188
F 2.023687391190 -3.149187190661 6.097193327794
F 3.463644603390 -4.691824344377 4.418005296575
F 4.248170457722 -3.718544230320 1.991231242135
F 3.566744053068 -1.179606308204 1.255549554153
F 2.108279013731 0.368237926919 2.915448326832
F 3.116185108553 5.346568415514 6.222942842285
F 5.156565037321 7.034458939352 6.732924636644
F 6.268088065553 7.131744211653 9.224367389129
F 5.322735261316 5.505917366385 11.202961136909
F 3.299596111167 3.796319263794 10.704007588875
F -3.315094738486 -3.235196896603 8.407491430893
F -5.502244510410 -4.807698916583 8.401632111405
F -7.882974946562 -3.849201994354 7.472067020353
F -8.048719066962 -1.291213964520 6.532592270136
F -5.863866082951 0.288228121607 6.505745946825
N 1.263620950507 1.585567051168 6.863735632386
N -0.300443822986 2.966655016067 8.604988594738
N -2.270582264823 1.483627207790 8.306310605354
N -0.982580960037 -0.210157253147 6.611472144236
Mn -0.661096245307 1.633692580065 7.230445212633
O -0.286847037449 -0.773117259790 10.348448392296
O -1.127403665401 -1.632369846623 10.284641775257
O -1.270052758235 2.647107930089 5.687884083292
H -2.184504590423 2.397063043684 5.478017565319

BP86-Optimized ¹[(TPFC)Mn^{III}(OH)(O₂)]-

C 1.237662213167 -0.560207127789 5.562231204466
C -0.104949496529 -0.967329014379 5.841349781034
C -0.833872621918 -2.071712462596 5.240785090855
H -0.449243570493 -2.752467600513 4.471101339382
C -2.097655126123 -2.081340809252 5.805032586255
H -2.917395811006 -2.772837336903 5.573400374184
C -2.160560942618 -0.982571433490 6.753014500955
C -3.297745061298 -0.595869292314 7.533894060189
C -3.327645103370 0.565750366063 8.364924043894
C -4.342197948485 1.097524576611 9.257514351300
H -5.336284590085 0.665779783816 9.431451417090
C -3.814619841452 2.242843078286 9.864683019736
H -4.313556596989 2.885837650896 10.600920857934
C -2.480522465156 2.409332072459 9.350685770922
C -1.345891621960 3.277077730110 9.514277575974
C -0.973694947383 4.468903664036 10.219524830111
H -1.610284268072 5.047495883273 10.901190422790
C 0.353069141124 4.756227633071 9.864673118936

H	0.950663722424	5.609384861479	10.210870099219	C	-0.965868883027	4.437099585163	10.240819742870
C	0.792573623574	3.730103069715	8.943826484420	H	-1.597968485366	4.997677357182	10.940927188228
C	2.027923796762	3.520990018313	8.254088159953	C	0.350654859156	4.736456976378	9.871250869679
C	2.251777703044	2.438570491485	7.353547839018	H	0.951360453094	5.585369628351	10.221879213731
C	3.488440120141	2.120326841623	6.669509495558	C	0.787823497705	3.723362910200	8.931073656735
H	4.426905199190	2.682017447163	6.756743263254	C	2.028409015008	3.530114251338	8.248775287771
C	3.273556917919	0.976866894460	5.918846326921	C	2.260799206066	2.446552166461	7.352439628671
H	4.008218652078	0.452064457073	5.295527135661	C	3.495359779624	2.118384933346	6.670373843900
C	1.896536200302	0.572899669976	6.124637770712	H	4.436004809054	2.676320109520	6.756143033275
C	2.016030311562	-1.393405500674	4.595961877294	C	3.273247644495	0.973136428178	5.923471482821
C	2.393777568735	-2.719375375843	4.899893604429	H	4.002436175618	0.442593765692	5.298915682315
C	3.121388170305	-3.516071598921	3.999002917545	C	1.894614980170	0.574808098945	6.130458916313
C	3.495885554659	-2.986607498623	2.751741600940	C	2.008864055225	-1.392563748600	4.605475385614
C	3.138737698554	-1.668710618602	2.417133626393	C	2.400605162948	-2.711929126528	4.919621081555
C	2.406905037045	-0.894775173532	3.334255753146	C	3.131845677540	-3.509275825690	4.022253387826
C	3.136861980136	4.489893451738	8.493530061531	C	3.495786175536	-2.986533471066	2.768981657013
C	3.617403012123	5.335628024689	7.469614988404	C	3.124373465633	-1.675152456571	2.424354524181
C	4.651244444909	6.262298684954	7.688559708060	C	2.388938563531	-0.900551343713	3.338060723922
C	5.229553750404	6.367720283753	8.965583768541	C	3.130513793436	4.504788293754	8.491793629665
C	4.773131793310	5.543159287775	10.008698564241	C	3.613637564356	5.347280251288	7.466202982924
C	3.740667618049	4.621525814724	9.763256305722	C	4.644363274008	6.277165786395	7.685857563105
C	-4.523299981782	-1.442477576907	7.467746173835	C	5.217104930304	6.388773261991	8.964886195815
C	-4.529689347139	-2.778511890789	7.927152411217	C	4.758329660039	5.567310964593	10.009452944007
C	-5.681058711914	-3.582759589705	7.874621752299	C	3.729638734187	4.641720054135	9.763344066796
C	-6.875834779524	-3.052004073181	7.357824344589	C	-4.549581666790	-1.446807874830	7.459792069040
C	-6.906485074127	-1.725013111250	6.894977509303	C	-4.569582468425	-2.786503903688	7.907433328794
C	-5.740598800332	-0.942380884768	6.954094686564	C	-5.730774256112	-3.576423369641	7.852244778642
F	2.071864475146	-3.254929677592	6.089759855831	C	-6.920994957300	-3.026414278516	7.345161681186
F	3.470070645712	-4.769885682370	4.323682796120	C	-6.938065077394	-1.694693541497	6.895092541209
F	4.190649266512	-3.734656639301	1.885773030207	C	-5.762540091745	-0.926871745009	6.956092288616
F	3.487171795546	-1.165340285966	1.223704822561	F	2.086382746431	-3.240337455724	6.114470305511
F	2.067712176203	0.353344549040	2.969140343743	F	3.493387151222	-4.756991551382	4.355497078401
F	3.073896545159	5.283665928912	6.241805699098	F	4.194063967046	-3.735054076651	1.906543867671
F	5.078465056643	7.055049234094	6.694887375498	F	3.463529550921	-1.178525894450	1.225636017237
F	6.212838665970	7.248436993324	9.186859911824	F	2.037301274853	0.341740521689	2.965635501686
F	5.331805122397	5.633898772402	11.224401775674	F	3.075084728120	5.288853356100	6.236647572692
F	3.347823636675	3.836517721390	10.780643151037	F	5.073886276484	7.066921143938	6.690995124372
F	-3.416438402716	-3.316368122393	8.453244448969	F	6.197190713175	7.272664524174	9.186796578814
F	-5.652592614390	-4.844701182235	8.327662657011	F	5.312032608529	5.663866899685	11.226816937337
F	-7.979450319268	-3.807647998727	7.305470453116	F	3.335261173255	3.858803226573	10.781615474450
F	-8.041692064549	-1.220516994848	6.389620782435	F	-3.460127017917	-3.341773078641	8.423179275953
F	-5.806171788543	0.312132120172	6.476250398310	F	-5.715551903763	-4.842760702981	8.292911163580
N	1.310995447338	1.471487699567	7.000285686573	F	-8.033631796028	-3.768188452521	7.290283374104
N	-0.255873705300	2.868464626083	8.765681579731	F	-8.069329208802	-1.171883599678	6.400135819570
N	-2.244264615885	1.392314228489	8.453440189519	F	-5.814170049425	0.333516258833	6.492903130407
N	-0.934387712100	-0.343457981666	6.737812605207	N	1.323829843778	1.484624894683	6.999690514156
Mn	-0.484165839024	1.334395795298	7.660549930587	N	-0.260295670150	2.862634128043	8.755996759353
O	0.002912753988	0.202182817389	9.084678214878	N	-2.225502162434	1.356657300150	8.468095566935
O	-0.515834930511	-0.860266834095	9.546641923160	N	-0.965695948989	-0.347784430263	6.730944832351
O	-1.158522654874	2.226862492780	6.222583727480	Mn	-0.508628844046	1.326097113591	7.598994774474
H	-2.134384461887	2.144426652744	6.227732066655	O	0.241348810406	0.227736345899	9.092895758186

BP86-Optimized ³[(TPC)Mn^{III}(OH)(O₂)]-t

C	1.228074632549	-0.556968693575	5.568475719505
C	-0.114293284553	-0.965362261959	5.839328090028
C	-0.832550439260	-2.078120324732	5.246504409781
H	-0.432770155678	-2.763920013650	4.489473523625
C	-2.102249962679	-2.096677079339	5.798443700956
H	-2.911402756713	-2.799969534340	5.565970374133
C	-2.188221529357	-0.998945563533	6.740894257781
C	-3.314195076732	-0.615752805348	7.526867211558
C	-3.313271583107	0.528873550960	8.381118197165
C	-4.313376765568	1.051700566578	9.287793407705
H	-5.304507330989	0.615128440737	9.465559681963
C	-3.783677046420	2.194909736892	9.900005968201
H	-4.276059534009	2.831236429492	10.645989091984
C	-2.460974074532	2.371563745000	9.375602548979
C	-1.337189950854	3.249258020145	9.524756718906

BP86-Optimized ⁵[(TPFC)Mn^{III}(OH)(O₂)]-

C	1.229785030105	-0.553408574714	5.570541717384
C	-0.113187406787	-0.954206590371	5.841888822517
C	-0.831906435837	-2.067865955271	5.253454334924
H	-0.430162021913	-2.762662253163	4.505747384726
C	-2.105963366247	-2.072870922638	5.794448201001
H	-2.916650794080	-2.775050092416	5.564167109410
C	-2.192071822272	-0.967532166466	6.727320454775
C	-3.319328859425	-0.594043037533	7.517042771397
C	-3.318440303021	0.535050674579	8.390672222333
C	-4.312530832553	1.039496689862	9.314629508650
H	-5.304835455276	0.603629619718	9.487519135937
C	-3.772771856802	2.164741521527	9.951073934245

H	-4.258103017398	2.786542617965	10.713828727658	C	-4.237957591449	1.003710229115	9.312741061467
C	-2.451960566420	2.346930112311	9.421724143701	H	-5.187072521457	0.509708850411	9.557289378065
C	-1.329172679334	3.227628913216	9.565131809703	C	-3.702605819570	2.138974328742	9.930340689110
C	-0.945630685553	4.396326113560	10.301737078781	H	-4.149201555565	2.718811283931	10.747937264076
H	-1.562825417068	4.936412066083	11.030726129085	C	-2.431686479416	2.384854064212	9.311275669066
C	0.362542232378	4.711404222083	9.910045209197	C	-1.311257856084	3.268488561224	9.452837311973
H	0.967354453636	5.553317807115	10.270313719779	C	-0.903237174581	4.381467774909	10.262292984551
C	0.781857282443	3.725934204435	8.936583735331	H	-1.502810805590	4.875443859786	11.037372278700
C	2.012101133611	3.543573702969	8.235149856531	C	0.404609856946	4.700697998168	9.878944944427
C	2.238272467619	2.465262366215	7.330311454646	H	1.032952056126	5.497338010132	10.297203002694
C	3.476089868833	2.143456310125	6.650539339007	C	0.796375364152	3.770323060517	8.841993947734
H	4.412316204998	2.709028143332	6.734684164133	C	2.032178678618	3.576058511763	8.157387386511
C	3.264813504460	0.989280244315	5.915251140104	C	2.249914169542	2.502482345299	7.245762772193
H	3.998964790578	0.457363077622	5.297711881332	C	3.504323819787	2.149287189008	6.614977384325
C	1.888752110210	0.584887358830	6.124848727244	H	4.454212830920	2.681861248273	6.748160004692
C	2.013804047047	-1.398165758154	4.618605660074	C	3.556788367372	-2.948424516035	2.723660154797
C	2.402321507695	-2.715062014433	4.946910366926	H	4.028112610245	0.451427399293	5.276554778620
C	3.137325936569	-3.521478617309	4.060800828250	C	1.891268062860	0.648687240059	6.015102077511
C	3.508462822926	-3.010733821044	2.804692321144	C	2.030311599097	-1.336455712205	4.513575777819
C	3.140269971309	-1.702199992721	2.446032573326	C	2.417309107153	-2.652456493062	4.848458471517
C	2.400920079804	-0.918371210612	3.348671601554	C	3.166079397261	-3.458786046963	3.973951048080
C	3.116557230239	4.516845904123	8.475201361255	C	3.556788367372	-2.948424516035	2.723660154797
C	3.579747932535	5.375543968673	7.454022524690	C	3.193600997260	-1.640011523575	2.359412802636
C	4.612582025580	6.304155155601	7.669199168080	C	2.439501373497	-0.856722390959	3.250083147242
C	5.208633277824	6.396699119238	8.939099442664	C	3.159506123381	4.512978803875	8.435739537244
C	4.770471020391	5.558148202599	9.978937234874	C	3.652347501065	5.385882529127	7.441017267721
C	3.738837639716	4.634543459296	9.737345553073	C	4.707791353781	6.280666537217	7.687529008495
C	-4.554312660117	-1.425862789792	7.441762284289	C	5.298662976679	6.321467194992	8.962544162454
C	-4.577134242154	-2.766722471200	7.885183362291	C	4.832502205935	5.465864963800	9.975942865904
C	-5.739201214471	-3.554965844852	7.824087302184	C	3.777958537822	4.577320998251	9.703258439251
C	-6.927364799677	-3.001467937384	7.315892214683	C	-4.487565899351	-1.459939279681	7.445137390115
C	-6.941589448980	-1.668146508367	6.870486532222	C	-4.446883123829	-2.795191526057	7.904488549498
C	-5.765222437208	-0.902024277414	6.937669315954	C	-5.583160897391	-3.622385056976	7.901639727498
F	2.081142782123	-3.232169996340	6.144850590836	C	-6.810528665628	-3.114806959513	7.441030794943
F	3.495571384599	-4.766463099206	4.407440981803	C	-6.888994689065	-1.787714169950	6.983792148275
F	4.210386492317	-3.767939602479	1.952875312865	C	-5.737414286919	-0.982196108969	6.991931657267
F	3.486199123979	-1.217048338536	1.244574183154	F	2.082780623050	-3.169091129590	6.043379573029
F	2.052255261022	0.320643695367	2.962686568495	F	3.521383424969	-4.702979899786	4.327492199481
F	3.020039978716	5.333164380061	6.233297723746	F	4.272501210292	-3.705584537430	1.882932401806
F	5.022973210856	7.109665920129	6.678904354850	F	3.558411421580	-1.154656337405	1.163374062343
F	6.191197541046	7.278882771015	9.156849168663	F	2.097156140958	0.382464257213	2.858522308917
F	5.346379907822	5.636735402648	11.187260291173	F	3.100372504069	5.390217558815	6.216102204641
F	3.364484874601	3.835094555674	10.750306259269	F	5.146035228516	7.101621462052	6.722084600140
F	-3.469659026492	-3.325016442021	8.401849170081	F	6.303102152913	7.170642825674	9.210154690672
F	-5.726858932861	-4.822852926739	8.260268174748	F	5.403676972012	5.494726935370	11.188830928876
F	-8.040785906939	-3.741571015509	7.255481842113	F	3.377926590309	3.759132116619	10.691355937159
F	-8.071051375925	-1.141843206006	6.375219041326	F	-3.300876861640	-3.311252329615	8.379977645093
F	-5.813980082561	0.360774582783	6.480913655586	F	-5.509063944197	-4.883990421848	8.350272742127
N	1.305959320532	1.495643427842	6.983852807696	F	-7.899865613697	-3.892513385672	7.436510816418
N	-0.269851222521	2.866780551468	8.756282355271	F	-8.056355463608	-1.304624400197	6.534122272415
N	-2.224879962437	1.351003230383	8.494131128892	F	-5.849170467407	0.273293392101	6.526130208142
N	-0.965280021529	-0.318261322975	6.721124785513	N	1.295045658193	1.568574558312	6.855123193594
Mn	-0.537530228924	1.372913749522	7.570935984851	N	-0.272737223884	2.943395516763	8.605128425572
O	0.293224380695	0.226691936814	9.123412583950	N	-2.231784967667	1.430057038238	8.333504765885
O	-0.367818306667	-0.763477993499	9.607463871412	N	-0.958379229895	-0.237052432410	6.599839863399
O	-1.182157350273	2.333012568797	6.132193112769	Mn	-0.633818515834	1.602321862746	7.237561765392
H	-2.004124089092	1.901478431273	5.820347689873	O	-1.180941221924	-0.030537149175	11.089487544388

BP86-Optimized $^7[(\text{TPFC})\text{Mn}^{\text{III}}(\text{OH})(\text{O}_2)]^-$

C	1.234815329890	-0.487009843843	5.450332383995
C	-0.104835063296	-0.889458169996	5.729409218511
C	-0.798250181361	-2.042021446306	5.190052782389
H	-0.385701932489	-2.754639793521	4.465411739920
C	-2.060629436428	-2.067591914559	5.755234701482
H	-2.852368740111	-2.803008431850	5.566532746723
C	-2.162594740923	-0.933734159711	6.650307056911
C	-3.282740887262	-0.582587806740	7.458012190684
C	-3.291022744198	0.562108836642	8.309523282700

C. $[(\text{TPFC})\text{Mn}^{\text{III}}]$

B3LYP-optimized

C	0.829611992207	-0.552686227471	5.191574288115
C	-0.479070691738	-0.978879396830	5.531442486691
C	-1.200965891383	-2.103539500358	4.994000505182
H	-0.830968533091	-2.785967913791	4.231921794206
C	-2.433556025870	-2.140770407567	5.601537766539

H	-3.228476799955	-2.859130381201	5.412394625483	C	-2.506952745135	-1.040417438639	6.529378881760
C	-2.508119294468	-1.041024212970	6.527426498097	C	-3.601191295743	-0.690114489952	7.356140282745
C	-3.602629665749	-0.690354173841	7.352324300600	C	-3.605676320056	0.458024165439	8.192018274732
C	-3.608693174588	0.458871117089	8.188126470927	C	-4.578570465750	0.975484611053	9.112650758596
C	-4.582264824439	0.978142303325	9.108667973319	H	-5.547957974304	0.529390758465	9.328132338760
H	-5.552891074275	0.534829738548	9.324306185082	C	-4.057503015592	2.136415385731	9.682415568034
C	-4.059780031796	2.137771323280	9.679413956727	H	-4.539014057836	2.772717023168	10.422431467426
H	-4.541921903234	2.773586080589	10.419971283272	C	-2.764509567024	2.330552421384	9.121585934218
C	-2.765611104302	2.330986376723	9.119235342369	C	-1.656466802429	3.225183582803	9.219070288028
C	-1.655676360499	3.224946819218	9.218969005290	C	-1.289379308243	4.434012353605	9.873334289133
C	-1.287436517704	4.432338204388	9.876778918603	H	-1.906518221700	5.002496188496	10.566394220573
H	-1.903700273646	5.000494302806	10.571456076962	C	0.000258920880	4.751340887394	9.449120086613
C	0.002591421968	4.749789288076	9.454312514523	H	0.582045616692	5.622021485874	9.746695265163
H	0.583746541211	5.619452910224	9.756068619175	C	0.430809751149	3.729840787088	8.536336000898
C	0.432927063792	3.730263128088	8.537549619017	C	1.634350702836	3.553193557637	7.803460482329
C	1.635925291474	3.553593169536	7.80226234407	C	1.849392857461	2.4690629259370	6.919334421098
C	1.849319314734	2.471810285175	6.916142224766	C	3.046424201267	2.176747219549	6.178665487411
C	3.044653822971	2.182255170811	6.167983453797	H	3.963341982753	2.761738744114	6.211294327097
H	3.961159549261	2.767946707202	6.194759643045	C	2.825992368794	1.030086877148	5.449939448969
C	2.824435491928	1.037507910714	5.439369358808	H	3.532992958841	0.528109827138	4.792676966719
H	3.531870459544	0.541317807655	4.778508774227	C	1.485260790343	0.587409986195	5.725010053634
C	1.484496859235	0.588719968120	5.719081057118	C	1.576271946819	-1.366119947172	4.195242348622
C	1.579112911366	-1.369188821445	4.190432705203	C	2.013139082804	-2.668060297614	4.481959384709
C	2.032989807484	-2.662148272486	4.486336756191	C	2.714530336149	-3.437490273967	3.551595509356
C	2.735452163776	-3.432560024702	3.558410578711	C	3.000144345145	-2.904586734450	2.292652785962
C	3.004868313346	-2.910285590178	2.292474541772	C	2.580634088802	-1.611141687100	1.974280782843
C	2.567680315524	-1.625879543836	1.965209264950	C	1.877666992167	-0.863148799772	2.920567164412
C	1.864134223212	-0.876415538263	2.909146012620	C	2.714775022178	4.562849418390	7.969769523006
C	2.717494995735	4.564930585231	7.971975151732	C	3.116997331300	5.392215458536	6.911034353935
C	3.106277949954	5.410583436076	6.922568951898	C	4.118856996669	6.352856843696	7.060380458476
C	4.106906050180	6.371077803548	7.076325183330	C	4.745169375791	6.508906286722	8.298843547968
C	4.746315884436	6.509575017451	8.309202249638	C	4.367445169350	5.702102555982	9.374362958786
C	4.381763302280	5.685659870571	9.375135830698	C	3.364975214554	4.746182000286	9.199979795938
C	3.379830118874	4.730618749453	9.197011296954	C	-4.802821544832	-1.567537730283	7.353470323676
C	-4.807032385425	-1.567864675272	7.351777082083	C	-4.747867423869	-2.891305389757	7.817618248518
C	-4.757653266465	-2.884982251837	7.832064078668	C	-5.869742156770	-3.721972491813	7.826185717884
C	-5.880763681545	-3.713071666404	7.842972540844	C	-7.094147282047	-3.231501580210	7.367220627088
C	-7.100631122619	-3.226945841543	7.370143727831	C	-7.185213925955	-1.917866716807	6.902048633961
C	-7.185483132787	-1.919689714259	6.888735082402	C	-6.048713792532	-1.106972225850	6.900053326318
C	-6.048088559094	-1.110967586956	6.884711486704	F	1.766638623517	-3.206013418273	5.680500347504
F	1.801534802157	-3.191972935606	5.689367242088	F	3.119767599987	-4.670528853808	3.859068205427
F	3.155556842258	-4.656333011169	3.874785055607	F	3.670059052490	-3.627710604544	1.398329052351
F	3.674870944875	-3.633771907436	1.401305345488	F	2.846491110168	-1.103434839045	0.769846480735
F	2.818250522855	-1.127270508552	0.755756610674	F	1.483244886506	0.367204176136	2.578004916135
F	1.455900094175	0.344714331761	2.557317024087	F	2.527764234717	5.284866925312	5.716208473025
F	2.508265663721	5.318946811072	5.732995481873	F	4.472069748729	7.128194434934	6.034411243994
F	4.447533503537	7.160732637984	6.059481791337	F	5.700187076945	7.422688559587	8.453216580271
F	5.699555436508	7.421840505947	8.467209202982	F	4.970735662040	5.843241382727	10.555292041720
F	4.995382269726	5.810303415192	10.550468681644	F	3.040344347030	3.982686805238	10.247947396374
F	3.067329782420	3.953779447405	10.236309414788	F	-3.597899239400	-3.390606060487	8.280927821200
F	-3.613390021667	-3.381789954742	8.306453879221	F	-5.782499499562	-4.973269433343	8.279164426207
F	-5.798164807880	-4.957521135301	8.309968994208	F	-8.170551755534	-4.013917656210	7.372407673214
F	-8.176942135986	-4.006254456777	7.377518586985	F	-8.351508620422	-1.450300130143	6.455247927545
F	-8.346323564183	-1.455368674192	6.430087596362	F	-6.170984152836	0.138953945871	6.431739802825
F	-6.166436277040	0.128164167313	6.403148439516	N	0.922711662074	1.474537796199	6.621464506831
N	0.926656679580	1.474088915121	6.617345115233	N	-0.594607700887	2.833055736393	8.430261909632
N	-0.593374272974	2.837543370005	8.432147972141	N	-2.534486876576	1.305941411772	8.226624578873
N	-2.540349067163	1.306992054626	8.225504671669	N	-1.296900838696	-0.356838199523	6.459165071440
N	-1.297994956481	-0.358602845522	6.452177952776	Mn	-0.826417824557	1.257827419495	7.379233512451
Mn	-0.827397145649	1.259212670775	7.377271314483				

BP86-optimized

C	0.828456785256	-0.552094080869	5.196286414027	C	0.834602660891	-0.557878822672	5.185671701511
C	-0.480826058126	-0.977921476398	5.533649399835	C	-0.480816757305	-0.983374561132	5.525746613502
C	-1.203146664486	-2.097126204389	4.990877234594	C	-1.205668844360	-2.106932032676	4.979186296137
H	-0.832490663168	-2.774621625997	4.224468488771	H	-0.831301499978	-2.787683547704	4.205253769407
C	-2.436952619956	-2.134762416588	5.599750110038	C	-2.447228461556	-2.146236391549	5.591916805709
H	-3.235814605571	-2.848616245339	5.409394021324	H	-3.252982028240	-2.864766127726	5.399112863448
				C	-2.516676038449	-1.048707191802	6.526430528280

C -3.616878369034 -0.699573179053 7.357556580204
C -3.616600758885 0.454006123949 8.195976699742
C -4.594069636712 0.972942789121 9.122276752534
H -5.569801867335 0.521141036963 9.340712237708
C -4.070042722705 2.141413479704 9.694593291576
H -4.554367886123 2.782720392839 10.441145051336
C -2.772183824824 2.335679576205 9.129371990577
C -1.661092557092 3.233212547021 9.227023206174
C -1.294273439999 4.447353846042 9.885057807047
H -1.916938672424 5.019500028686 10.583725052681
C 0.002691051063 4.767751487128 9.457675315900
H 0.589022144634 5.645867894526 9.755975589840
C 0.435297825976 3.741058149939 8.540243630699
C 1.645620411515 3.567886568542 7.806301496260
C 1.859576107068 2.477791824794 6.918257405530
C 3.061843616794 2.184035761638 6.175844338128
H 3.986406200774 2.772852093468 6.210386804797
C 2.839205248791 1.030128939989 5.442742230545
H 3.551239717466 0.522340481874 4.781115369074
C 1.492223294543 0.586984311065 5.718472286567
C 1.584887198410 -1.375234586962 4.183130591267
C 2.038500577929 -2.677540239154 4.482252014841
C 2.745301302590 -3.453750035820 3.547533336331
C 3.017447936939 -2.925576835288 2.273160839277
C 2.579928662917 -1.630646483754 1.943429229174
C 1.872228128163 -0.875962689891 2.894767936385
C 2.728163908994 4.580267865820 7.975732984785
C 3.122019115658 5.425617477865 6.915484557125
C 4.130133035223 6.392725570595 7.068818821648
C 4.769567274505 6.536522560542 8.312813912796
C 4.399241182095 5.711950321982 9.389832602432
C 3.389965842802 4.750307508024 9.211135182729
C -4.822771052790 -1.577397437673 7.355891454258
C -4.770084617022 -2.905041828920 7.834232246141
C -5.900901580173 -3.739362486506 7.843296489588
C -7.130007614583 -3.246463067341 7.370651503098
C -7.217405115398 -1.927697440966 6.890859821081
C -6.071781420737 -1.113522681737 6.888831720889
F 1.806724133892 -3.207582352527 5.694310058463
F 3.167870657627 -4.685511671980 3.8638811632854
F 3.690787798927 -3.653807619433 1.375912824229
F 2.832795711453 -1.130054987544 0.726332979884
F 1.458702863980 0.352423011590 2.542868894880
F 2.519000119681 5.330195695304 5.719394605431
F 4.476389849415 7.184354344277 6.044742367117
F 5.729010024417 7.454506435788 8.470811263072
F 5.015118807226 5.841893014369 10.572640936096
F 3.073378373566 3.968837566870 10.256495329226
F -3.617985745283 -3.402960895942 8.311949971711
F -5.819084881689 -4.992937428527 8.309286963176
F -8.213091269719 -4.030719248548 7.376342170900
F -8.386175324792 -1.460616113182 6.431456469878
F -6.187757030601 0.134072254550 6.405299864233
N 0.924332772993 1.479225247913 6.619984270608
N -0.593577771868 2.837153753585 8.431703690694
N -2.538407382365 1.305213581294 8.227828173066
N -1.300448096822 -0.358225138805 6.458390592387
Mn -0.826207467439 1.257978811539 7.377577955080

D. O₂

B3LYP-optimized

O 0.060232631343 -0.722379593664 0.000000000000
O 1.259767375311 -0.722379593664 0.000000000000

TPSSh-optimized

O 0.058490305788 -0.722379593664 0.000000000000
O 1.261509700865 -0.722379593664 0.000000000000

BP86-optimized

O 0.051865156259 -0.722379593664 0.000000000000
O 1.268134850395 -0.722379593664 0.000000000000

E. OH

OH-radical

O 0.007917434510 0.000000000000 0.000000000000
H 0.992082565490 0.000000000000 0.000000000000

OH-

O 0.009036734100 0.000000000000 0.000000000000
H 0.990963265900 0.000000000000 0.000000000000

F. THF

TPSSh-optimized THF

C 3.773102702157 -2.433083045577 9.091042962501
O 3.487444408717 -1.076124493159 9.451477890616
C 4.25651527656 -0.179748999482 8.640360491981
C 5.305226698636 -1.041802469386 7.936579518976
C 4.550125456393 -2.366053569500 7.775432676219
H 4.378568208661 -2.908379840010 9.886919240370
H 2.824168308364 -2.987981213550 9.008856247572
H 3.593138601764 0.317850357506 7.906473462324
H 4.693701212746 0.599533778775 9.285713412178
H 5.645052967479 -0.608404070512 6.984464458601
H 6.186363190671 -1.180830922660 8.584546724019
H 3.855581077125 -2.308100096140 6.921168711393
H 5.208224639629 -3.234210416306 7.623646203249

THF-radical

C 3.176018023322 -2.246393545560 8.847006672735
O 3.115412552934 -1.488866706991 9.994693731897
C 3.699779220945 -0.204383248748 9.710063647873
C 4.753603273568 -0.490118431165 8.640119364301
C 4.090370489801 -1.623163758343 7.827636179626
H 3.023194455076 -3.316058239287 9.012239659036
H 2.914133099277 0.477171299370 9.335783575082
H 4.100024372975 0.196986515422 10.651082179689
H 4.998569550324 0.397230177704 8.039376804840
H 5.678903717478 -0.853561711345 9.114473871514
H 3.527186217129 -1.210165245587 6.968092727925
H 4.821931027172 -2.336041105471 7.412471585483

G. [(TPFC)Mn^V(O)]

Singlet [(TPFC)Mn^V(O)]

C 0.783394880403 -0.583990174114 5.259022042999
C -0.514055068912 -0.979969326824 5.611699740006
C -1.245995838631 -2.066650368031 5.034760570446
H -0.883016825442 -2.713925500239 4.239791735371
C -2.466309610713 -2.112642436219 5.658896229088
H -3.287358099473 -2.796649808552 5.456078129366
C -2.504683308438 -1.049135915520 6.617293056978
C -3.616185623255 -0.715159763059 7.412113039727
C -3.598761785446 0.428241823226 8.218662773302
C -4.616525449589 1.022541674200 9.032825360475
H -5.614698352679 0.616922828851 9.184694772059
C -4.099830948226 2.190118623966 9.574075718867
H -4.606951365329 2.897314582814 10.226911393101
C -2.764111070350 2.300883673260 9.103134323544
C -1.672010899206 3.177640984690 9.199216021209
C -1.348473769370 4.434279010608 9.776706646847
H -2.008330114774 5.043325153439 10.390811672447
C -0.053238097049 4.732064781671 9.378968494339
H 0.518722010525 5.624777031180 9.624309159670

C 0.412904201352 3.653949446309 8.559271209877
 C 1.616421543416 3.480976664727 7.866070358892
 C 1.799524894040 2.377040831142 7.014509039017
 C 2.975822504266 2.113831350135 6.241129542937
 H 3.879670772655 2.718544269170 6.257294978027
 C 2.742307326773 0.986377522377 5.496956832501
 H 3.423289722045 0.496956433476 4.804614375367
 C 1.420544298166 0.534764386200 5.810598553411
 C 1.512258988246 -1.381051380609 4.231662150697
 C 1.967006214783 -2.679643326488 4.501902775163
 C 2.653493379371 -3.434979647148 3.549355160845
 C 2.899451255267 -2.890799858150 2.286603216072
 C 2.457455557579 -1.600443100678 1.985603438331
 C 1.772488002974 -0.864552689524 2.954264984087
 C 2.691176756582 4.498282876545 8.010938110345
 C 3.082651837449 5.317248406859 6.940979602398
 C 4.078268998229 6.286077970165 7.077720828680
 C 4.705687016501 6.459589722709 8.313594344847
 C 4.336088482836 5.663315119210 9.399927293747
 C 3.338418242846 4.700089386793 9.239366286102
 C -4.834832562433 -1.566182475019 7.362042032820
 C -4.825445798163 -2.882317216694 7.848105829520
 C -5.961411465985 -3.692539329004 7.809776227445
 C -7.149523748984 -3.187734736354 7.276129015284
 C -7.191840537668 -1.881390753853 6.783906607850
 C -6.042755951573 -1.089813252707 6.831400940000
 F 1.751222822459 -3.224946428842 5.702014423902
 F 3.078356847867 -4.664973302775 3.837720427038
 F 3.553262256794 -3.600781499332 1.371561370868
 F 2.687276895341 -1.083447096322 0.778767172578
 F 1.358098760921 0.364446700653 2.634775093371
 F 2.491025463082 5.188733676051 5.750220097811
 F 4.424565174761 7.051509489000 6.043051515948
 F 5.654438188635 7.380648879074 8.455290192196
 F 4.938818474921 5.823991797171 10.577723504015
 F 3.013562627361 3.950119078441 10.295939433077
 F -3.707187312443 -3.391262988576 8.372279729809
 F -5.921847975411 -4.937221836386 8.284649526422
 F -8.238194339841 -3.950505167227 7.235560830428
 F -8.322782868306 -1.401901184416 6.266759990232
 F -6.113865520353 0.149998531499 6.338870274171
 N 0.851085140197 1.384457176362 6.752515146582
 N -0.590022563438 2.715418433441 8.479317259687
 N -2.475197719811 1.222250905733 8.293754549500
 N -1.293414594978 -0.356682853320 6.576645996061
 Mn -0.646247063698 0.915552343114 7.877911072932
 O -0.057492399533 0.052632080558 8.993500637180

C 1.611389261792 3.474818921985 7.915691240900
 C 1.798017882881 2.366598291354 7.024535384773
 C 2.983443755756 2.109854848800 6.265629413347
 H 3.890233708890 2.710065487250 6.284581537200
 C 2.763433770564 0.964221742020 5.530297295216
 H 3.461234754574 0.473803408353 4.855575453432
 C 1.439656607922 0.517281084308 5.837688535700
 C 1.535798985328 -1.410130116650 4.264216325254
 C 1.950576372266 -2.728907363886 4.504460561405
 C 2.641453930848 -3.470474303573 3.544721794510
 C 2.924876591668 -2.895978350041 2.303289085239
 C 2.519645381787 -1.586888295305 2.031452623958
 C 1.835356873151 -0.861579280923 3.007887841681
 C 2.675617267263 4.507582543695 8.007178883710
 C 3.049647526762 5.286759236863 6.990330608396
 C 4.032986729200 6.272562051556 6.990826631583
 C 4.669585539393 6.501198991429 8.213376306908
 C 4.319138975442 5.744455452704 9.333975361755
 C 3.328643956530 4.767383648700 9.223041569359
 C -4.842934175092 -1.545155364823 7.346942675886
 C -4.845414776765 -2.881610874442 7.777082868352
 C -5.991406217078 -3.675102929486 7.715790604690
 C -7.175852285308 -3.135451253166 7.207784925030
 C -7.205370783593 -1.810196590265 6.767577481119
 C -6.048319688429 -1.032744896620 6.842301408721
 F 1.701408789821 -3.302508580246 5.683830282055
 F 3.033756568879 -4.716346862364 3.805967124524
 F 3.579361016595 -3.594255431911 1.381261695649
 F 2.781644719578 -1.043039588723 0.844020828104
 F 1.449449160738 0.382033164328 2.712990899774
 F 2.444052263281 5.110936181240 5.723608734471
 F 4.358074095276 7.002941058080 5.925491395180
 F 5.607848870440 7.437027566354 8.309714566810
 F 4.932053649165 5.95648975689310 4.97345269954
 F 3.026637897738 4.05497048015310 3.10612094977
 F -3.731114241792 -3.421523040401 8.276693977600
 F -5.965098558694 -4.936444487170 8.143023858621
 F -8.273022697697 -3.882569963839 7.143534940221
 F -8.331746943553 -1.299081502957 6.273038978833
 F -6.108056143791 0.223735832969 6.394305335845
 N 0.867438909840 1.380386467206 6.750477597573
 N -0.531389952706 2.690813154900 8.644187749844
 N -2.479958408664 1.226575103596 8.310260249637
 N -1.267231838214 -0.485886183714 6.619123655192
 Mn -0.655462372283 0.908633025653 7.854703597702
 O -0.053900211891 0.055229851675 9.030725433250

Quintet [(TPFC)Mn^V(O)]

C 0.794630523421 -0.590299360771 5.256952895726
 C -0.522687756483 -1.012460192558 5.583242321734
 C -1.266058109115 -2.086261820585 4.980791269008
 H -0.917652104355 -2.726262382435 4.173383028402
 C -2.498381144678 -2.119468286400 5.594556623695
 H -3.323637248467 -2.791510823651 5.369959275191
 C -2.519058502847 -1.066450368300 6.573829231217
 C -3.626496068842 -0.709409533637 7.419182870641
 C -3.621121650520 0.410232645580 8.267656524058
 C -4.640091375932 0.994807451781 9.109903336367
 H -5.642588956556 0.600596542387 9.263637310070
 C -4.112848521063 2.152950792977 9.659815160810
 H -4.612789429848 2.849569743538 10.329287287111
 C -2.772098290080 2.265390159036 9.167841202510
 C -1.647052855923 3.173455402139 9.264010720645
 C -1.331917553827 4.443047412172 9.848150256871
 H -1.990517259866 5.046405405187 10.469166171026
 C -0.043051126138 4.754982033383 9.443504193905
 H 0.511701355555 5.661362093697 9.678175288347
 C 0.426404549675 3.669136524657 8.613501576310
 C 1.612453245000 3.493518013093 7.878601539962

Triplet [(TPFC)Mn^V(O)]

C 0.798408349736 -0.632064025623 5.298525385248
 C -0.496192991835 -1.076833134881 5.645315995668
 C -1.249912697141 -2.127328628862 5.013314785361
 H -0.907940810418 -2.751617161283 4.190790972060
 C -2.485589179023 -2.146507272352 5.615890006980
 H -3.327512838228 -2.789675459177 5.369039582488
 C -2.486157133851 -1.109853144734 6.614483430545
 C -3.609222160072 -0.719138176557 7.417333842182
 C -3.596431933829 0.425960048230 8.223977957893
 C -4.617350158297 1.012665006385 9.056655188978
 H -5.619702644304 0.616278233018 9.206223794343
 C -4.089259136375 2.164173346589 9.620543766302
 H -4.588303164410 2.85632774233010 2.95188556728
 C -2.746971678653 2.267661995596 9.147334121205
 C -1.619374423676 3.154150902711 9.296106168112
 C -1.339392983348 4.452644030512 9.836841475198
 H -2.025851693212 5.07679591006710 4.05146185778
 C -0.044533649982 4.760737197549 9.454187688432
 H 0.494360608001 5.684824383866 9.654881511500
 C 0.446906750989 3.643936364634 8.679587997102

C 1.835213467096 2.387594784020 6.987533398346
 C 3.027816822752 2.124337896781 6.229281096180
 H 3.935461005276 2.723375443621 6.245613934978
 C 2.804231363594 0.981717009632 5.493390797917
 H 3.498135065756 0.495550725814 4.811558475974
 C 1.471166212949 0.537647957796 5.797220532194
 C 1.527315147469 -1.398061234054 4.240782407811
 C 1.922780964753 -2.717662812660 4.506708512495
 C 2.610965204808 -3.484070250180 3.564777982680
 C 2.912472042630 -2.933410776238 2.316729199161
 C 2.527665807165 -1.623524846560 2.020347305077
 C 1.845326649887 -0.873210207023 2.979251259721
 C 2.679938722152 4.519843265732 8.008367928450
 C 3.079829748626 5.307161921585 6.916612622811
 C 4.069387972878 6.283737129512 7.034616305588
 C 4.686205323778 6.493680271035 8.270584087093
 C 4.310330141551 5.727548774574 9.376484310353
 C 3.314686702353 4.759124967077 9.237683283999
 C -4.846745289039 -1.557873724093 7.358173920929
 C -4.820962175448 -2.895660490131 7.782446830390
 C -5.955743886774 -3.706222520665 7.736131320896
 C -7.156400570550 -3.182224870133 7.250320441129
 C -7.213705317308 -1.855458693297 6.817326992419
 C -6.067525551913 -1.060705605297 6.876885415522
 F 1.655446993016 -3.267676271139 5.693198929837
 F 2.983967761702 -4.730630772646 3.849249193053
 F 3.565037821384 -3.655313442381 1.411846542950
 F 2.807811179819 -1.102093582277 0.827171019876
 F 1.480931853594 0.371566031064 2.662974245894
 F 2.494054421275 5.146600611491 5.727653208431
 F 4.419418397707 7.022199759427 5.982998612789
 F 5.630013421716 7.420693496536 8.393604007491
 F 4.904603608815 5.921826024728 10.552440385865
 F 2.988407041455 4.036508599893 10.311389061872
 F -3.690299069480 -3.420083491209 8.261041359347
 F -5.903118403043 -4.968871401501 8.156567349255
 F -8.242848164059 -3.945746126059 7.200519549430
 F -8.356033800806 -1.359077302840 6.345297419500
 F -6.153075011279 0.197824489544 6.439401346577
 N 0.916908610897 1.407451528503 6.707616581771
 N -0.581077025671 2.744206544766 8.548589518140
 N -2.514748772115 1.214666446402 8.353202379415
 N -1.315881420544 -0.411272360143 6.532370397576
 Mn -0.701839643470 1.005363979437 7.715338533367
 O -0.046506327199 0.078911873170 8.896076785623

H. [(TPFC)Mn^V(O)(OH)]⁻

singlet [(TPFC)Mn^V(O)(OH)]⁻

C 1.618629508383 -0.057134848575 5.189133487322
 C 0.389294565193 -0.649063297959 5.593415894904
 C -0.257677119385 -1.820286724996 5.037260339083
 H 0.117927044094 -2.426995553040 4.215145808362
 C -1.432799035191 -1.997373777570 5.728012625551
 H -2.181107152263 -2.769824658720 5.558635253948
 C -1.524236984172 -0.937396702735 6.711924891084
 C -2.609201752990 -0.686635700447 7.599096867644
 C -2.688638987336 0.449122653033 8.451117097337
 C -3.704333347190 0.894787961674 9.380990750371
 H -4.634195007478 0.374489673907 9.606143614756
 C -3.273676694285 2.093650093677 9.935047052696
 H -3.801813698652 2.702100234459 10.667393050963
 C -1.991949169899 2.381051561811 9.355230734332
 C -0.968330193121 3.380249617289 9.413316117502
 C -0.736860176831 4.656088862858 10.007412851821
 H -1.407091014942 5.181012057400 10.686377854987
 C 0.497640215283 5.106142521326 9.539449122304
 H 0.975354760778 6.054976231843 9.779440178254
 C 1.022179787572 4.100041561154 8.656870213774

C 2.190349576186 4.054400016171 7.848644294481
 C 2.456239429166 3.006513834774 6.933596775907
 C 3.599991158851 2.881001571829 6.064371121213
 H 4.440343188070 3.571558409778 6.023931958403
 C 3.434329103998 1.739964899691 5.315508312579
 H 4.120323705476 1.344924306042 4.568639652393
 C 2.182960629052 1.136025972959 5.709077203874
 C 2.373210889713 -0.749864803372 4.105086817247
 C 2.957721398147 -2.009350286116 4.308237051966
 C 3.659452928450 -2.676678444742 3.302347570667
 C 3.795066173817 -2.081992365304 2.046324579946
 C 3.227347893724 -0.828600028684 1.808488024354
 C 2.526515348753 -0.184310155965 2.829990681457
 C 3.151986340458 5.185039095368 7.946341374018
 C 3.397186416477 6.050798804736 6.868418662730
 C 4.27347090213 7.122364120874 6.961826202779
 C 4.956014974993 7.361600624026 8.164008007840
 C 4.731568986409 6.524818987329 9.259102718289
 C 3.840184208986 5.456979988441 9.139737476159
 C -3.740232786587 -1.653476831556 7.615066749423
 C -3.570573176502 -2.979358522604 8.044959734860
 C -4.624510940269 -3.894564189665 8.071986550141
 C -5.898248714991 -3.492154297489 7.665153908380
 C -6.104171806939 -2.180589451068 7.232745717344
 C -5.033198890962 -1.285071628262 7.210518576532
 F 2.861707555931 -2.606239196510 5.501310258725
 F 4.207773519043 -3.871330744559 3.534996288592
 F 4.463863595507 -2.707532141566 1.078868397838
 F 3.348567439585 -0.261302783713 0.606214697949
 F 1.984827805268 1.007708735792 2.557160307349
 F 2.757832046463 5.874820545896 5.707164774575
 F 4.490435588426 7.927390379374 5.916845420654
 F 5.805014445507 8.382734522455 8.265262586560
 F 5.376004913859 6.744882791497 10.406932068122
 F 3.666808668369 4.669689677854 10.206603201161
 F -2.371469363411 -3.399487732337 8.462130793444
 F -4.425992802265 -5.144817389725 8.495016213247
 F -6.912023962727 -4.355769806528 7.688535216580
 F -7.317678104659 -1.795641086033 6.831845064918
 F -5.269438028850 -0.045872569690 6.766192877828
 N 1.636390007342 1.916200418538 6.703119839037
 N 0.120437283922 3.078907989799 8.630110053625
 N -1.698709558249 1.377708488461 8.485158137004
 N -0.400540497451 -0.160756142446 6.585136460808
 Mn 0.056839159245 1.449818986137 7.669265373341
 O 0.634163459545 0.455362585164 8.722860825194
 O -0.878400870118 2.308697014319 6.271359708221
 H -1.752857972538 1.901106064244 6.162352905251

triplet [(TPFC)Mn^V(O)(OH)]⁻

C 1.599063457972 -0.030298690906 5.154309115078
 C 0.364573402804 -0.614214116123 5.552633665457
 C -0.271954017825 -1.793207634258 5.007480670187
 H 0.118496286500 -2.404235335628 4.195845751105
 C -1.455802590127 -1.977652819938 5.683699031431
 H -2.189642341125 -2.763302221441 5.513131367103
 C -1.575941758530 -0.918056041868 6.658687678782
 C -2.644271145085 -0.679614060989 7.560918963499
 C -2.709180989921 0.454374176736 8.419198186106
 C -3.666406875914 0.840709077227 9.625789769123
 H -4.561396352419 0.283000834125 9.697532371958
 C -3.234575877293 2.038259329192 9.987956302986
 H -3.723616431727 2.602609005398 10.780115699242
 C -2.012015968440 2.385446024019 9.333564456683
 C -0.991528591921 3.387124766802 9.390541312473
 C -0.729121206201 4.636691134213 10.030710261619
 H -1.370201547041 5.134640991721 10.756110142590
 C 0.490320680457 5.094680540895 9.539248406034
 H 0.986446392438 6.027460841975 9.803099872140

C	0.981663514542	4.120827226145	8.598098695509	H	0.993634296421	6.035875084057	9.827119432468
C	2.153419698320	4.090136313156	7.791932012211	C	1.003791922187	4.100385617986	8.648121071810
C	2.431041602482	3.056827568049	6.860188192026	C	2.154780752468	4.063978059562	7.828160494484
C	3.614729678719	2.890356134909	6.049108255974	C	2.451332727808	3.015724477223	6.894590921305
H	4.474241714458	3.558134997312	6.041828671622	C	3.621579973617	2.888713008294	6.053456759285
C	3.457974449785	1.738647255823	5.313893482506	H	4.461889711574	3.579646081624	6.024613879815
H	4.169236485558	1.311933379017	4.609220207349	C	3.474028546541	1.737421486017	5.316044890863
C	2.173133613639	1.170619564545	5.659411488024	H	4.173029744263	1.333224944885	4.586684848290
C	2.371125370112	-0.751600326956	4.102136052679	C	2.208757749977	1.147120661085	5.696409733454
C	2.934342764071	-2.015541310635	4.337426923965	C	2.370309916420	-0.759279109296	4.118196099527
C	3.657364586446	-2.703095587462	3.360716117616	C	2.939053325492	-2.022052751218	4.341180065404
C	3.839546649129	-2.124339706480	2.103123458015	C	3.648140625778	-2.700659190372	3.348401595479
C	3.295420904173	-0.866817658579	1.833988921538	C	3.800245816572	-2.116088952607	2.089204398796
C	2.571658837421	-0.202373535610	2.826087825408	C	3.244347504234	-0.860625732565	1.833647148731
C	3.131722266717	5.201073927980	7.932441934923	C	2.541097802058	-0.200468021922	2.843059998408
C	3.417887709897	6.074110457883	6.870240271432	C	3.119485769194	5.192821011784	7.933183670203
C	4.329088491381	7.124495056782	6.994529151133	C	3.357828255806	6.060121880146	6.855605706748
C	4.981043213595	7.332320257162	8.211674256530	C	4.251793073368	7.128053128725	6.947725650937
C	4.718126555933	6.486088909121	9.290849955689	C	4.935549972705	7.353345993688	8.144567944342
C	3.806269894584	5.439589886340	9.140922005383	C	4.721194845596	6.509488017749	9.236371630297
C	-3.758674397497	-1.662595983490	7.612633241904	C	3.820834027179	5.448561048289	9.121784854047
C	-3.555406806106	-2.990530306126	8.021910135389	C	-3.745560114119	-1.652660329478	7.616057202370
C	-4.596621302320	-3.918546569748	8.083421162335	C	-3.571277828288	-2.983709726860	8.025095712633
C	-5.890970325340	-3.527549130328	7.734778745845	C	-4.625760010692	-3.898107925847	8.040961721625
C	-6.130653391406	-2.214157542425	7.325695396673	C	-5.898605707668	-3.488846306118	7.636914963132
C	-5.072393945122	-1.305458180829	7.268009083257	C	-6.105549594123	-2.171852751402	7.221282842985
F	2.796423437124	-2.597041297928	5.533806525311	C	-5.036029754861	-1.274328145557	7.215224075002
F	4.183413090243	-3.901399791300	3.623529335713	F	2.821910061941	-2.605833339676	5.537231406067
F	4.529813521337	-2.769121018963	1.163935722944	F	4.184288642160	-3.896329788237	3.595671724477
F	3.461212715164	-0.314782327227	0.630022406189	F	4.473449886132	-2.753890139653	1.134953675880
F	2.053784622342	0.992882653000	2.523454388920	F	3.382505066006	-0.304919213238	0.629338190110
F	2.797503242125	5.926146653543	5.695011765248	F	2.012430248447	0.993516711483	2.559984683994
F	4.569320270934	7.938281744441	5.964460097684	F	2.706235321835	5.888139205325	5.701840715771
F	5.850447647987	8.332589394612	8.342377802842	F	4.447453798332	7.939007422902	5.907499029324
F	5.347938334218	6.674766831317	10.452192602013	F	5.789555759091	8.368800223877	8.243597283921
F	3.600835301698	4.639416564315	10.192315845593	F	5.380321267349	6.717421850379	10.376719038892
F	-2.335907035272	-3.400106255388	8.386591099672	F	3.654676706230	4.653935757331	10.182810156616
F	-4.365976709580	-5.170096493061	8.485162491498	F	-2.370097659597	-3.405112300516	8.431077647560
F	-6.892422040046	-4.403562676183	7.791546430394	F	-4.428143919704	-5.153048293210	8.445888321737
F	-7.364448755035	-1.840062346594	6.980970400988	F	-6.911292910939	-4.351777564730	7.647712162155
F	-5.341466794621	-0.064374598783	6.849287396009	F	-7.317783916856	-1.782349127912	6.825283984547
N	1.597719202853	1.997866921469	6.586508352064	F	-5.269216965652	-0.028670494100	6.791871469781
N	0.061244332806	3.117405850747	8.557444915069	N	1.641539859421	1.943850457167	6.652506024349
N	-1.751510724806	1.422673651023	8.398158653537	N	0.085364659934	3.092150022767	8.613098293112
N	-0.455618976344	-0.130118678819	6.535575386994	N	-1.674791127840	1.348010520772	8.520263863683
Mn	-0.062427953189	1.541846660536	7.463715955276	N	-0.420334352324	-0.152156167957	6.586954196015
O	0.733325265228	0.477193888740	8.578394148502	Mn	0.026341479512	1.448432448096	7.600390217459
O	-0.918474674283	2.437259505931	6.062864768967	O	0.905107367708	0.572232922621	8.751191746450
H	-1.872416680655	2.270624267862	6.147799840046	O	-0.935319746898	2.409096717349	6.142774626271
				H	-1.838150850851	2.051935213600	6.149006121744

Quintet [(TPFC)Mn^{VI}(O)(OH)]⁻

C	1.616360345772	-0.047036847583	5.190898342076
C	0.377347636093	-0.632137889945	5.585608312642
C	-0.271934982650	-1.791735885976	5.012715145405
H	0.102717861157	-2.386129060291	4.181781705310
C	-1.451266434373	-1.974307145677	5.695890925493
H	-2.199793675668	-2.743522521934	5.515691895136
C	-1.537249689547	-0.929368974749	6.693188358653
C	-2.611784207144	-0.687712775577	7.612464356108
C	-2.678621621627	0.422019474380	8.485155347961
C	-3.692089066249	0.860000177115	9.422648541958
H	-4.624740934004	0.343494323573	9.642834736196
C	-3.257870629810	2.055996727096	9.972762479675
H	-3.778826769318	2.665769780553	10.708785792513
C	-1.977352321975	2.342360837301	9.382121171850
C	-0.952898380727	3.366305085331	9.428992260446
C	-0.709712609953	4.637213868639	10.060383042583
H	-1.363001046012	5.139309396360	10.771825817716
C	0.504617503091	5.096496829074	9.574524875919

[(TPFC)Mn^{VI}(O)(OH)]

C	1.598237236207	-0.030229749063	5.159258393919
C	0.350626786876	-0.606862859427	5.540652825225
C	-0.293445984905	-1.765762893311	4.976078231213
H	0.089309240935	-2.366290610554	4.154055558608
C	-1.478671459058	-1.948057552318	5.653369266737
H	-2.222751162468	-2.720700822201	5.473191717452
C	-1.577426642822	-0.903281720784	6.640074233626
C	-2.651057201984	-0.665692216019	7.562685628947
C	-2.718195547183	0.457459972452	8.414027490167
C	-3.671268590128	0.840885378761	9.429939304008
H	-4.562407302278	0.280714933687	9.706107657677
C	-3.238716975138	2.034351907549	9.986869175392
H	-3.718058849386	2.600826309767	10.782183205534
C	-2.017927943375	2.378893613072	9.320734595151
C	-0.984838522173	3.388115781537	9.328433178976
C	-0.731723013300	4.643861454017	10.026385452615
H	-1.381262365264	5.138956750981	10.744769208109

C 0.483916873480 5.099538426451 9.542054238184
H 0.978973899674 6.032744548606 9.803425201759
C 0.982403237868 4.117602476836 8.604210240946
C 2.144884818276 4.082405474794 7.808849160344
C 2.438404892222 3.030106776693 6.874808769307
C 3.631165269027 2.865943222269 6.082652738487
H 4.492502164565 3.530062675732 6.088113433536
C 3.478889310343 1.714237773503 5.343915179541
H 4.195582360618 1.284074244735 4.648038522076
C 2.189961725272 1.159101845545 5.675497949459
C 2.366407185599 -0.752060482676 4.105374865172
C 2.900676039884 -2.028557303529 4.338057740708
C 3.625224414106 -2.713154290525 3.361248695553
C 3.825080546822 -2.121749121030 2.111465670069
C 3.302728956720 -0.853113740988 1.847875255854
C 2.585510912713 -0.184241982094 2.841052217952
C 3.122781406642 5.193977057077 7.937621550862
C 3.415914310861 6.039604572943 6.855499183717
C 4.324796448078 7.092293631462 6.967124410159
C 4.970290812905 7.318946491389 8.185353173923
C 4.701696657206 6.944695352118 9.280698117064
C 3.785456856169 5.450003713678 9.148843905999
C -3.755024137620 -1.658708945356 7.615522727933
C -3.523385900512 -2.989252099207 8.000466762841
C -4.553571065217 -3.927985065768 8.065913448627
C -5.856203631421 -3.545292465286 7.736001630910
C -6.119076814210 -2.229976225326 7.345907632161
C -5.075077834140 -1.305239772040 7.292592584211
F 2.735442573530 -2.614442829388 5.526048281000
F 4.129772063123 -3.919503566180 3.614454720711
F 4.511792526480 -2.765696888034 1.173646291104
F 3.487283422453 -0.293357684993 0.653447463396
F 2.090063474446 1.022040844887 2.556165892816
F 2.801316479642 5.860950139756 5.683973186886
F 4.572068544441 7.885349970308 5.926173329239
F 5.838305209839 8.318057946490 8.301759168382
F 5.324523980803 6.704737486986 10.439045313355
F 3.565121564309 4.671566972160 10.210569835798
F -2.292984003551 -3.381066159551 8.338663158776
F -4.305034936178 -5.179314955700 8.447795878165
F -6.844101526475 -4.431702267886 7.793483389696
F -7.359004360023 -1.868205034501 7.021332293624
F -5.358585965663 -0.061592773039 6.899464521126
N 1.607629195483 1.983653782595 6.602464531635
N 0.056872161726 3.111244265850 8.563348630156
N -1.756786101376 1.432139942921 8.387812078093
N -0.461113277092 -0.123594870273 6.533243541306
Mn -0.067327973693 1.537681118852 7.462160248996
O 0.736574081847 0.522173860722 8.621734589932
O -0.873350115496 2.461428795769 6.068379985195
H -1.839935439062 2.369517434097 6.123798539904

I. [(TPFC)Mn^{III}(OH)]⁻

B3LYP-optimized [(TPFC)Mn^{III}(OH)]⁻

C 0.508229235882 -0.356998180339 4.363281179252
C -0.731258614534 -0.738744146195 4.942505283354
C -1.568000082412 -1.848107346456 4.546097862827
H -1.362611260523 -2.538068382923 3.730074077487
C -2.636501816528 -1.886738906917 5.408237985363
H -3.445828517647 -2.614478104337 5.410747137443
C -2.478022447058 -0.806409753490 6.352933613074
C -3.317556993995 -0.518920345881 7.457409706996
C -3.016850342473 0.482476751799 8.420361246788
C -3.651020957381 0.848347478262 9.661193814695
H -4.561400672293 0.410143155661 10.067127868242
C -2.874580601981 1.838722763214 10.255869174325
H -3.057594751846 2.325552558732 11.212749647870

C -1.775354161533 2.084786945631 9.377194215297
C -0.580099150524 2.870336840102 9.334431048200
C 0.115099101367 3.824973604840 10.138276978584
H -0.214698205024 4.224755141141 11.096160299194
C 1.295085226950 4.132965922957 9.466868639008
H 2.069175354002 4.820941153839 9.803261331174
C 1.323235212489 3.355053349845 8.254553955011
C 2.302673885477 3.217184487494 7.233147359250
C 2.180972840231 2.295362288569 6.164597459256
C 3.161057738192 2.028398175785 5.138711434211
H 4.126512655788 2.521590997231 5.042852324554
C 2.663803274951 1.032974171602 4.333778577189
H 3.152338301546 0.591251159048 3.467820039660
C 1.368938598867 0.659422371795 4.854954360529
N 1.109830175555 1.444664902373 5.950511718865
N 0.173226653118 2.628322304692 8.217264390644
N -1.911591723095 1.266311955514 8.288098280838
N -1.313267886429 -0.133969935583 6.027326112145
Mn -0.661110030336 1.553278596356 6.814466119909
C 0.952584870732 -1.112019424446 3.154135901299
C 2.048489527088 -1.986320884684 3.185302648234
C 0.284458070625 -0.987041947733 1.927342961573
C 2.467335941322 -2.696506538120 2.059002616694
C 0.679872577054 -1.689945066056 0.788251740582
C 1.778431293043 -2.547875920175 0.854615944123
C -4.551354195103 -1.334497181633 7.642818713627
C -4.702228410917 -2.211518333580 8.726938750858
C -5.624184495497 -1.256830179779 6.742401667184
C -5.857837264962 -2.971810532307 8.913084313696
C -6.788064175395 -2.009598828860 6.905095636539
C -6.905646784975 -2.870351602034 7.997179096063
C 3.526437656777 4.064765332385 7.308002285729
C 4.464298337958 3.918196046937 8.340507876819
C 3.790339768006 5.060360599300 6.355662251165
C 5.605209821934 4.717455565562 8.428271037878
C 4.926037760656 5.869043363759 6.419448122783
C 5.836779714632 5.697997107748 7.462824551671
F 6.921186811790 6.464554224056 7.535645325326
F 6.477430608940 4.544348781825 9.420936656209
F 4.290769967459 2.980744901805 9.275629070622
F 5.140199343088 6.808633689755 5.498900399236
F 2.936886381708 5.267281772289 5.349758917443
F -5.557494086721 -0.435752682062 5.691651631508
F -7.789151134548 -1.905262561119 6.031598059738
F -8.010664565743 -3.591549265605 8.163483481335
F -5.962402130256 -3.799963088306 9.952046999349
F -3.716560838216 -2.354087864956 9.616583592007
F 2.726666789625 -2.169249363378 4.321378478097
F 3.512160404565 -3.521440960247 2.128441462832
F 2.166594893142 -3.221334585781 -0.224901275274
F 0.022408737549 -1.541177082359 -0.361739481740
F -0.765519057850 -0.169074864460 1.818613868896
O -1.537026511230 2.877582962944 5.679398271104
H -0.899757670965 3.543825654921 5.386393296908

TPSSH-optimized [(TPFC)Mn^{III}(OH)]⁻

C 0.508891604160 -0.356939774001 4.368475139485
C -0.731049542806 -0.739210109455 4.946484082194
C -1.567409477860 -1.844969802911 4.546822320232
H -1.360314133548 -2.531900758727 3.728326700148
C -2.637209603222 -1.884131272852 5.410086512414
H -3.449215776833 -2.609179925555 5.413445645531
C -2.475050440144 -0.807934245621 6.356094860425
C -3.314043132305 -0.521664994176 7.462546099290
C -3.007423662393 0.471528169929 8.431086515095
C -3.648496689152 0.843469319667 9.665264055298
H -4.566959144745 0.413198359214 10.061600098441
C -2.868325319260 1.827247024614 10.266455042806

H	-3.055214127479	2.317918025683	11.220274053546	C	-2.884944391108	1.839731923752	10.276685382729
C	-1.759820927698	2.062873149348	9.397327046741	H	-3.075161822379	2.337951757878	11.235804090706
C	-0.564054729690	2.845532332657	9.356469047239	C	-1.769032226334	2.073145737650	9.404646727452
C	0.124241786227	3.811877389236	10.151617747371	C	-0.569825827104	2.857912864580	9.363733998128
H	-0.209316307600	4.217581411629	11.105359294227	C	0.119095823362	3.832637880349	10.160949991657
C	1.300675172626	4.124073164761	9.475628199705	H	-0.219640118144	4.244486246743	11.120096405821
H	2.070197166604	4.821526889485	9.803170771512	C	1.302323816587	4.146398753728	9.481124115561
C	1.333144546347	3.337260235907	8.270435545784	H	2.076908010835	4.851687943546	9.808497215602
C	2.306687967192	3.208897274158	7.243225407316	C	1.336999203082	3.351957541879	8.272078269887
C	2.183375103846	2.289712525842	6.171269476019	C	2.318447440043	3.224071558756	7.244601661264
C	3.159780008632	2.030029565653	5.142819203538	C	2.194012994326	2.298636914719	6.168203866549
H	4.123291381128	2.527561112658	5.047574889908	C	3.175069538430	2.037027810512	5.136510068524
C	2.660854984541	1.035181849159	4.335049805126	H	4.146569727115	2.537785310909	5.041406749161
H	3.144495657830	0.595864820192	3.464782004348	C	2.671167436258	1.036797533073	4.323385996754
C	1.371277038907	0.658019588891	4.860560879633	H	3.157396115857	0.593165132234	3.446024756110
N	1.11916486895	1.437604363536	5.962378335771	C	1.375871206521	0.659321202877	0.659321202877
N	0.190591709188	2.594494747523	8.239516254854	N	1.114340699507	1.444072036959	5.959392663185
N	-1.889623423649	1.242591761593	8.305850429173	N	0.189655678817	2.601288327879	8.240304222294
N	-1.308801259854	-0.134905767512	6.036079714695	N	-1.895753403898	1.245552035648	8.307082921124
Mn	-0.642055031340	1.526866518263	6.842767476563	N	-1.312940008338	-0.140073432874	6.037516502495
C	0.950593515364	-1.108764767204	3.159347259823	Mn	-0.642019540574	1.525301317318	6.845211133799
C	2.057860167051	-1.970652304845	3.183135101444	C	0.954522434307	-1.115711146030	3.144312531666
C	0.268875587491	-0.996338971898	1.937614447999	C	2.063550624330	-1.988888350039	3.171588809773
C	2.475072549595	-2.679832994050	2.054945109101	C	0.273070307678	-0.993682210298	1.913710347231
C	0.661957304590	-1.698640770588	0.796697596523	C	2.484260404060	-2.701531156418	2.035358115022
C	1.772243538115	-2.543357521588	0.856125518353	C	0.668783418556	-1.699585804894	0.764522997118
C	-4.551704377351	-1.329247962220	7.637793981262	C	1.781736406435	-2.556259487472	0.826367119453
C	-4.720902121783	-2.199206048032	8.726252199271	C	-4.570732035352	-1.339629966042	7.647542162808
C	-5.613107961023	-1.253523565283	6.722014851935	C	-4.733800338195	-2.219070308977	8.740046269085
C	-5.882290365235	-2.954106116743	8.902087960345	C	-5.642597472004	-1.256231444960	6.731879943368
C	-6.782486100368	-2.001016776193	6.873750138696	C	-5.902943165570	-2.978172079070	8.920724856588
C	-6.917766159040	-2.854357298828	7.970697916534	C	-6.819964650149	-2.007789441566	6.887826998806
C	3.522870557178	4.064027614905	7.307437819350	C	-6.950416626689	-2.871582312283	7.989268092285
C	4.462409278958	3.938350706736	8.342609749411	C	3.538026473458	4.080416087922	7.313135116670
C	3.781205937659	5.048149555808	6.340088172080	C	4.484858661458	3.941770155183	8.351339714761
C	5.599129153242	4.745691200449	8.418550759560	C	3.793784914465	5.079406441307	6.348263682912
C	4.912595128919	5.864556381099	6.391424847410	C	5.629751264839	4.753157683834	8.432983502126
C	5.824801617733	5.713610938055	7.437775437602	C	4.933332883345	5.900177271565	6.404652955366
F	6.906454809035	6.488407008366	7.499166355113	C	5.854111249419	5.737136013059	7.454346186475
F	6.474777139584	4.591240532842	9.413924058905	F	6.941582902761	6.514775948839	7.520706198472
F	4.294843093663	3.010098934461	9.290784426168	F	6.513353795026	4.588074282711	9.428228921825
F	5.120929033255	6.794383610819	5.456877105732	F	4.319199000702	2.997364076027	9.293054685460
F	2.923069670306	5.237118676806	5.331946259693	F	5.140979912869	6.8444335373590	5.475257708083
F	-5.529339215448	-0.435942000674	5.667221299968	F	2.926269738709	5.281231513902	5.342049536420
F	-7.773689621197	-1.897567092081	5.985981386966	F	-5.563810503426	-0.427006351418	5.677592771673
F	-8.029326912826	-3.571293497149	8.127144764294	F	-7.821906711586	-1.898302745558	6.003214061699
F	-6.003861964980	-3.777482431560	9.945509024834	F	-8.067641339590	-3.591100488609	8.149742870776
F	-3.744588927836	-2.341592659529	9.629141464905	F	-6.020918731242	-3.810897019164	9.965325147551
F	2.747129379677	-2.143415375123	4.316467286570	F	-3.745844192592	-2.369123557029	9.638644770511
F	3.530900392421	-3.494445185579	2.117289495616	F	2.748077387494	-2.172331656064	4.313842815035
F	2.158891804149	-3.216862185621	-0.226308401440	F	3.539577911534	-3.527251197170	2.098850987997
F	-0.007950407569	-1.561118781526	-0.349791441397	F	2.170719217699	-3.231932305517	-0.262118689446
F	-0.792153705029	-0.188423038792	1.836725583513	F	0.002168563791	-1.553766144202	-0.390377981337
O	-1.508119870151	2.863330563144	5.729978077562	F	-0.785403130783	-0.172002079098	1.810354261949
H	-0.844841838574	3.495111919789	5.408319843220	O	-1.497482519875	2.847017802638	5.711264957829
				H	-0.811727776256	3.446138992537	5.355143323940

BP86-optimized [(TPFC)Mn^{III}(OH)]⁻

C	0.511793784503	-0.362903236934	4.356961022010
C	-0.732810876199	-0.747811007283	4.941035844833
C	-1.569575931764	-1.861718301819	4.541914162283
H	-1.357885834200	-2.555025871903	3.718536996613
C	-2.645358007243	-1.903525825951	5.411585799040
H	-3.462246650421	-2.635896131667	5.417634882653
C	-2.483682453450	-0.820410898505	6.358913157249
C	-3.329950515960	-0.530736995140	7.468601224001
C	-3.021328409760	0.471147373522	8.435336935554
C	-3.668540123914	0.848879630918	9.673339856649
H	-4.595965619956	0.416853595375	10.070457602503

³RC

C	1.328486171453	-0.381493786017	5.101642061844
C	0.020140143334	-0.857566780585	5.384207112144
C	-0.668400522918	-1.957197309965	4.750504206188
H	-0.268797650231	-2.575795624258	3.949251410538
C	-1.910113384646	-2.059706749842	5.333142070703
H	-2.690481889927	-2.776887547405	5.085580457898
C	-2.011204699797	-1.029290035439	6.337647203529
C	-3.116862316463	-0.754265160024	7.179197992852
C	-3.139965043188	0.324965915144	8.104267086863

C -4.114118966235 0.729277816506 9.082671244686
H -5.067160278196 0.236597287653 9.269133265155
C -3.613535014837 1.844419356329 9.751253692522
H -4.095885768558 2.394333411942 10.557364611793
C -2.332891715184 2.123492464833 9.190012490666
C -1.242736645645 3.030113704826 9.364763310802
C -0.896070331942 4.176941277672 10.142828497969
H -1.520181574444 4.657806647368 10.893974738467
C 0.385251675063 4.555221994636 9.753013435483
H 0.957889305309 5.397396439646 10.138375784821
C 0.827449758562 3.632586040311 8.737829266404
C 2.042005336258 3.535309750414 8.004684962731
C 2.283907326896 2.529708714034 7.035922792803
C 3.504153074858 2.298106199637 6.304593375563
H 4.416270071011 2.884241504117 6.400175404450
C 3.308872354043 1.201042673382 5.496896192427
H 4.034925439062 0.746253022088 4.825762730565
C 1.960874568463 0.734502708409 5.712957462367
C 2.110700258819 -1.119937750694 4.069454913911
C 2.553432766710 -2.434928541755 4.279965048258
C 3.283945151124 -3.137497266576 3.319574576637
C 3.596537312185 -2.522337057604 2.105584264957
C 3.174482641415 -1.213552850462 1.862809071788
C 2.441259764182 -0.534198156125 2.837657848659
C 3.114005189923 4.530195172878 8.276461184370
C 3.537623018747 5.444370177154 7.298462502356
C 4.539692852036 6.385164356860 7.543462867901
C 5.146022358981 6.436038979310 8.800330063491
C 4.747689831984 5.543898154772 9.797991207187
C 3.745492244082 4.610415921954 9.527638827640
C -4.309134514027 -1.639233839287 7.103317390097
C -4.246676498533 -2.997929099241 7.452735158648
C -5.363513041209 -3.833623426546 7.393469328817
C -6.593078520204 -3.314501065771 6.983059024987
C -6.693208884211 -1.966540210502 6.632560528722
C -5.561291822791 -1.151816154772 6.695608641373
F 2.286539754000 -3.053289681253 5.435178717574
F 3.693458717627 -4.385373362086 3.557226012600
F 4.295064707887 -3.181395003951 1.182730949665
F 3.465342199859 -0.626334397628 0.700058040302
F 2.043225873848 0.712371239424 2.562285530795
F 2.969099044619 5.441595808638 6.088374286936
F 4.911543121175 7.242577116665 6.591069524468
F 6.101194048015 7.330649993604 9.046044910030
F 5.332371723189 5.582551590265 10.996728541483
F 3.407080759894 3.761673845068 10.505229086345
F -3.094374610875 -3.529985513464 7.873109818622
F -5.267003626319 -5.118854419855 7.739374676277
F -7.665450958201 -4.101911902382 6.925196269556
F -7.864410486728 -1.469578001782 6.229890741979
F -5.695262765285 0.128125801281 6.332284481396
N 1.380960512976 1.557610839318 6.646862752609
N -0.183824195275 2.743723926080 8.544489091028
N -2.097433561474 1.196777358757 8.203309266025
N -0.821506509705 -0.330235693865 6.329920583789
Mn -0.424116954900 1.305032807047 7.281031452070
O 0.425382847554 0.141660356748 8.706039554727
O -0.224038442260 -0.875934269029 9.138828479960
O -1.103530671658 2.382227212970 5.934889636407
H -2.068063841108 2.258632033212 5.914957982674
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F 4.295600149415 -3.856424563385 2.234232879411
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¹IM2

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¹TS3

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