Proton-assisted activation of a Mn^{III}–OOH for aromatic C–H hydroxylation through a putative [Mn^V=O] species

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Materials and methods:

All the commercially available chemicals used in the study were used as purchased. Hydrogen peroxide was purchased from TCI Chemicals, and triethyl amine was acquired from Alfa Aesar. Mn^{II}(H$_2$O)$_6$(ClO$_4$)$_2$ from Sigma Aldrich and HPLC grade solvents (MeCN, MeOH, and H$_2$O) were availed from Thomas Baker.

Caution! Perchlorate salts of metal complexes containing organic ligands are potentially explosive. These compounds should be prepared in small quantities and handled with proper safety precautions.

Instrumentation:

Agilent 8453 diode-array spectrophotometer was used to record UV/Vis absorption spectra. The -40 ˚C temperature was maintained with a cryostat from Unisoku Scientific Instruments. 1 cm quartz cells (λ = 190-1100 nm range) were used to monitor reaction kinetics on the UV/Vis spectrophotometer. ESI-MS was performed using Agilent 6546 LC/Q-TOF under positive ion mode. Resonance Raman spectra were obtained at 405 nm excitation wavelength (40 mW, Cobolt lasers, HÜBNER Photonics) using Kymera 328i motorized Czerny-Turner Spectrograph (Andor Technology) equipped with a DU 420A-BEX2-DD camera (iDus 420 CCD, Andor Technology). The CCD camera was cooled to -80 ºC. The spectral slit width of the instrument was set to 100 μm. The spectral calibration was performed using a 1:1 MeCN: toluene (v/v) solvent mixture. NMR spectra were recorded on a Bruker 400 MHz spectrometer at 233 K. The X-band electron paramagnetic resonance (EPR) was measured on a JES-FA200 ESR spectrometer at 77 K in acetonitrile solution. EPR parameters : [frequency, 9136 MHz; power, 0.995 mW; field center, 490.0 mT, width, ± 500.00Mt; sweep time, 30.0 s; modulation frequency, 100.00 kHz, width, 1 mT; amplitude, 1 mT; and time constant, 0.03 s].

The reaction mixture was injected (10 μL) in HPLC system (Agilent 1260 infinity machine model) attached with a ZORBAX SB-C-18 reverse phase column (150 × 4.6 mm, 5 μm) and DAD detector. Individual purity of the sample was analyzed prior to reactivity studies using HPLC experiments with the method described below: A gradient mixture of water and acetonitrile possessing 0.1% trifluoroacetic acid (pre-degassed by applying vacuum and ultrasonication) was used as the mobile phase. Method: 0 min to 15 min, 0.5 mL per min flow rate. For the oxidation reaction of xanthene, the condition given in the table below was used.

Time (minutes)	Water (0.1% trifluoroacetic acid)	Acetonitrile (0.1% trifluoroacetic acid)
0.00	70.00	30.00
5.00	70.00	30.00
5.10	40.00	60.00
8.00	40.00	60.00
8.10	10.00	90.00
12.00	10.00	90.00
12.10	70.00	30.00
15.00	70.00	30.00

Method of detecting formaldehyde in the solution:

The presence of formaldehyde in the solution is detected using the Hantzsch reaction.[1] The reaction between acetylacetone, ammonia, and formaldehyde at pH 6 results in a yellow-colored species due to the formation of diacetyl-dihydro-lutidine at room temperature. The yellow species gives a prominent band at 412 nm in the UV/Vis spectrum.[1]

The reagent solution is prepared by mixing of NH_4OAc (15 g, 0.19 mol), acetic acid (0.3 mL, 5.4 mol), and acetylacetone (0.2 mL, 1.9 mol) in 100 mL water.[2] Addition of reagent solution to the solution of **3A** in MeOH, depicted a band at 412 nm, confirming the presence of formaldehyde in the solution.

Characterization of [(BnTPEN)Mn^{III}-(OO)]$^+$ (2):

According to the reported literature, the suitable way of generating Mn^{III}-OOH is via the protonation of Mn^{III}-(OO) species.[3] Hence, we first tried to synthesize [(BnTPEN)Mn^{III}-(OO)]$^+$ species. When 10 eq. of H_2O_2 and 2 eq. of triethyl amine were added to a solution of **1** in MeOH, a blue-colored species (**2**) with an absorption maximum at 600 nm ($\varepsilon_{600\,nm}$ = 240 M^{-1}cm^{-1}), and a shoulder at 380 nm is observed in the UV/Vis spectrum (Fig. 1 and S1). [H_2O_2] dependent studies show that the maximum yield of **2** requires 10 eq. of H_2O_2 and 2 eq. Et$_3$N (Fig. S2). A similar absorption spectrum was reported for [(MeTPEN)Mn^{III}-(OO)]$^+$ in MeCN at -25 °C.[4] ESI-MS studies on the formed species **2** revealed a signal at m/z = 510.17 with the formulation of [(BnTPEN)Mn^{III}O$_2$]$^+$, confirming its presence in the solution (Fig. S3). The perpendicular mode EPR spectrum of species **2** was observed to be silent (Fig. S4). This silent characteristic of the EPR spectrum of **2** confirms the oxidation state of Mn to be +3. The NMR studies revealed the paramagnetic shifted signals in the range of -50 to 100 ppm further validating the +3 oxidation state (*i.e.*, S = 2 system) of **2** (Fig. S5).[5] Based on the similarities in the UV/Vis spectrum of [(MeTPEN)Mn^{III}-(OO)]$^+$ along with ESI-MS, paramagnetic NMR, and EPR analysis, we assigned blue-colored 600 nm absorbing species in the present work to be a [(BnTPEN)Mn^{III}-(OO)]$^+$ (**2**) species.
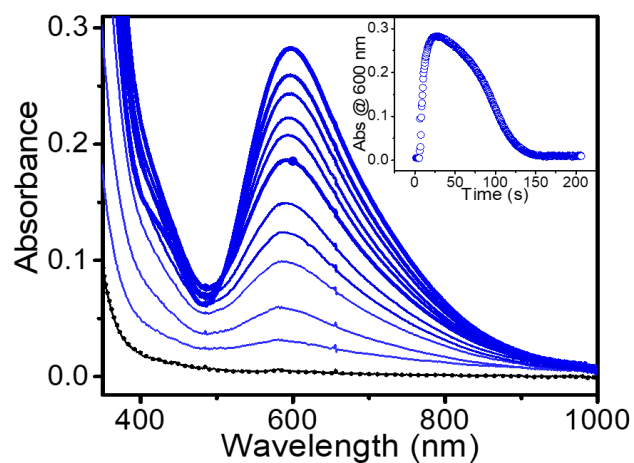
Figure S1: UV/Vis absorption spectral changes showing the formation of **2** (blue) by the reaction of **1** (black) with 10 eq. of H_2O_2 and 2 eq. of Et_3N in MeOH at room temperature. The inset shows the change in absorbance at 600 nm with time.
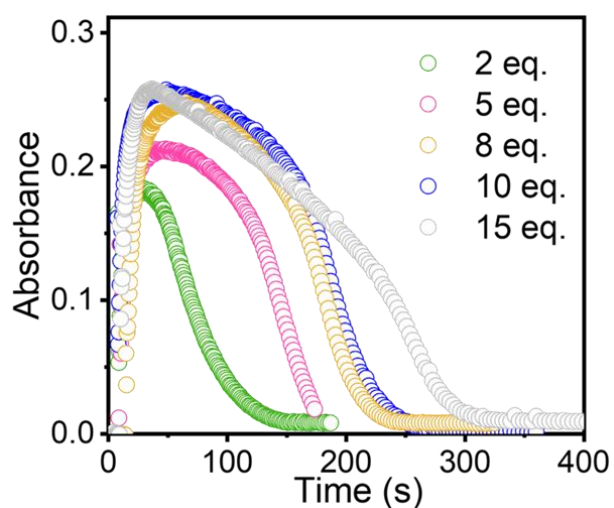
Figure S2: Absorbance vs time plot monitoring the formation and decay of 600 nm (**2**) species with different equivalents (2-15 eq.) of hydrogen peroxide and 2 eq. of Et_3N in MeOH at room temperature.
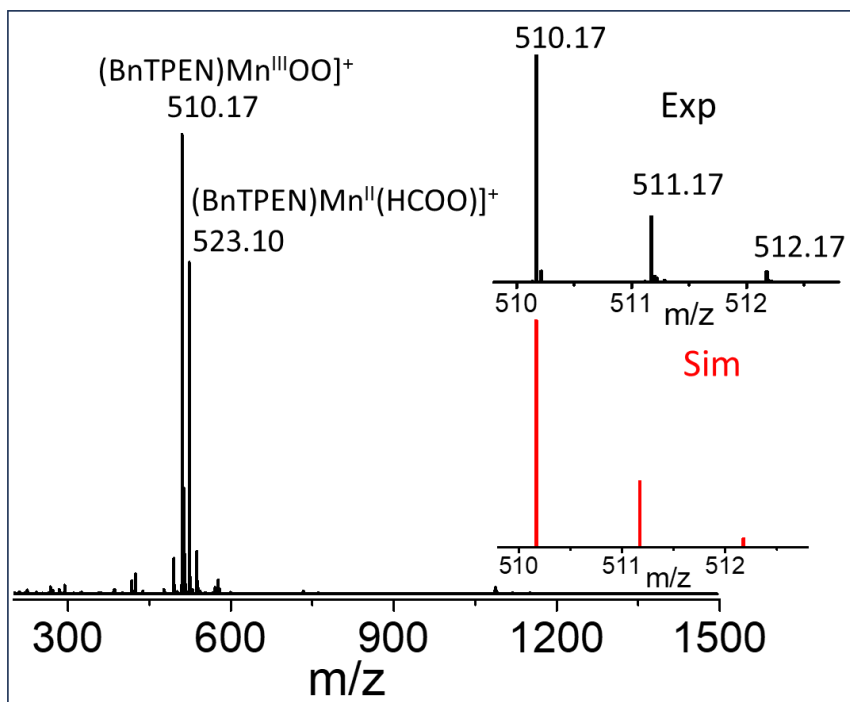
Figure S3: ESI-MS data of **2**, generated by the reaction of **1** with 10 eq. of H_2O_2 and 2 eq. of Et_3N in MeOH at room temperature. Note: The observation of a signal at m/z 523.10 for [(BnTPEN)Mn(II)(HCOO)]$^+$ alongside **2** likely arises from the ESI-MS conditions employed. Formate has been utilized as an ion to facilitate the acquisition of ESI-MS data.
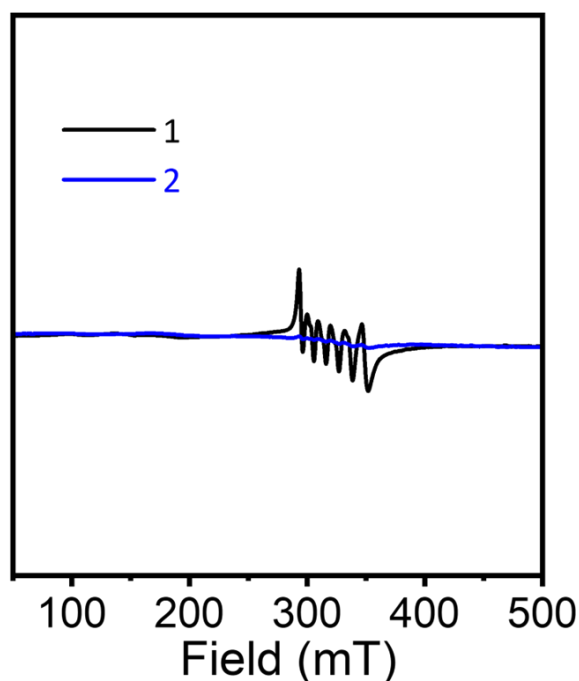
Figure S4: Perpendicular mode EPR spectra of **1** (black) and **2** (blue) in MeOH at 77 K. *Conditions to prepare 2*: 2 mM **1** in MeOH + 2 eq. Et_3N + 10 eq. H_2O_2 at room temperature.
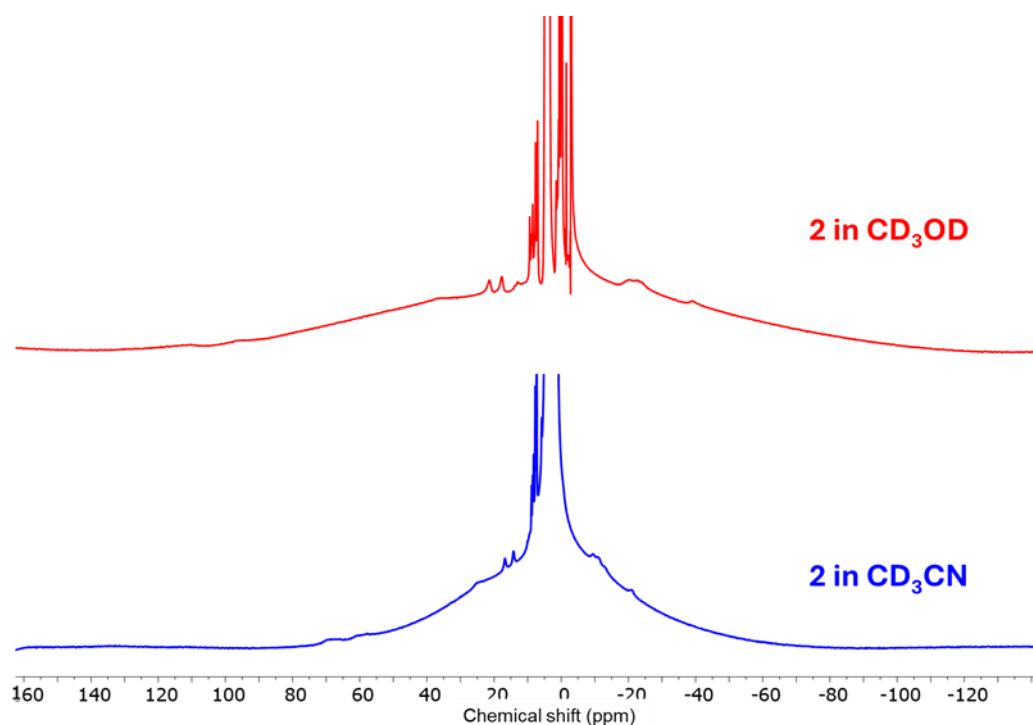
Figure S5: . ^{1}H NMR (400 MHz) spectra of **2** in CD_3CN (blue trace) and in CD_3OD (red trace) at -40 °C. *Conditions to prepare 2*: 4 mM **1** in CD_3OD/CD_3CN + 2 eq. Et_3N + 10 eq. H_2O_2.
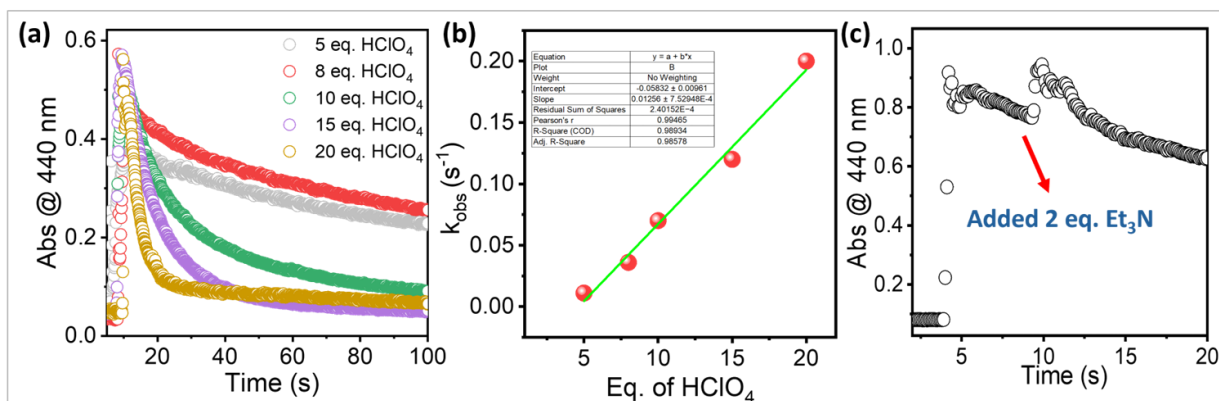
Figure S6: (a) Absorbance vs time plot monitoring the formation and decay of 440 nm (**3A**) species with different equivalents of (5-20) $HClO_4$ in MeOH at -40 °C. (b) Linear dependence on [$HClO_4$] of the decay rate of 440 nm species at -40 °C. (c) Absorbance vs time plot monitored at 440 nm showing the addition of 2 eq. Et_3N to **3A** in MeOH at -40 °C. Note: The addition of 2 eq. of Et_3N to **3A** did not result in the regeneration of **2** from **3A**. This suggests that an excess of Et_3N (approx. 4 eq.) is necessary to drive the equilibrium (Figure S7).
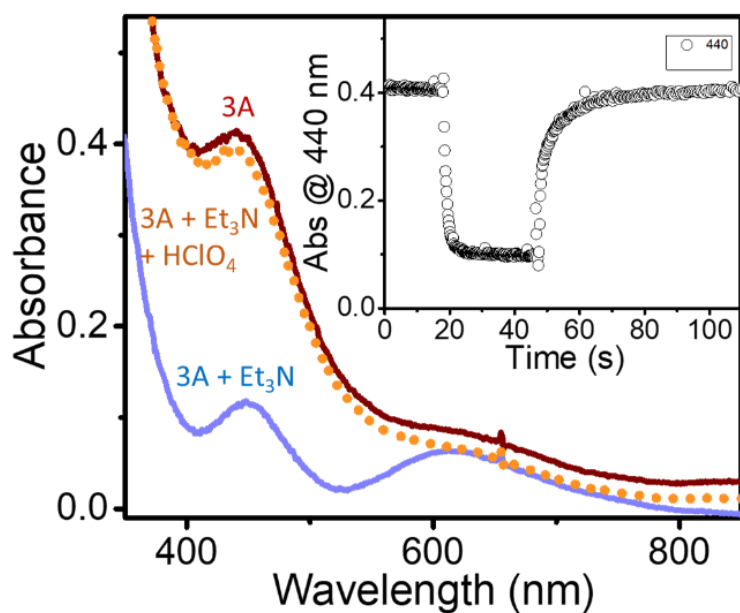
Figure S7: UV/Vis absorption spectral changes showing acid-base equilibrium between **2** and **3A** in MeOH at -40 °C. The inset shows the change in absorbance at 440 nm vs time.
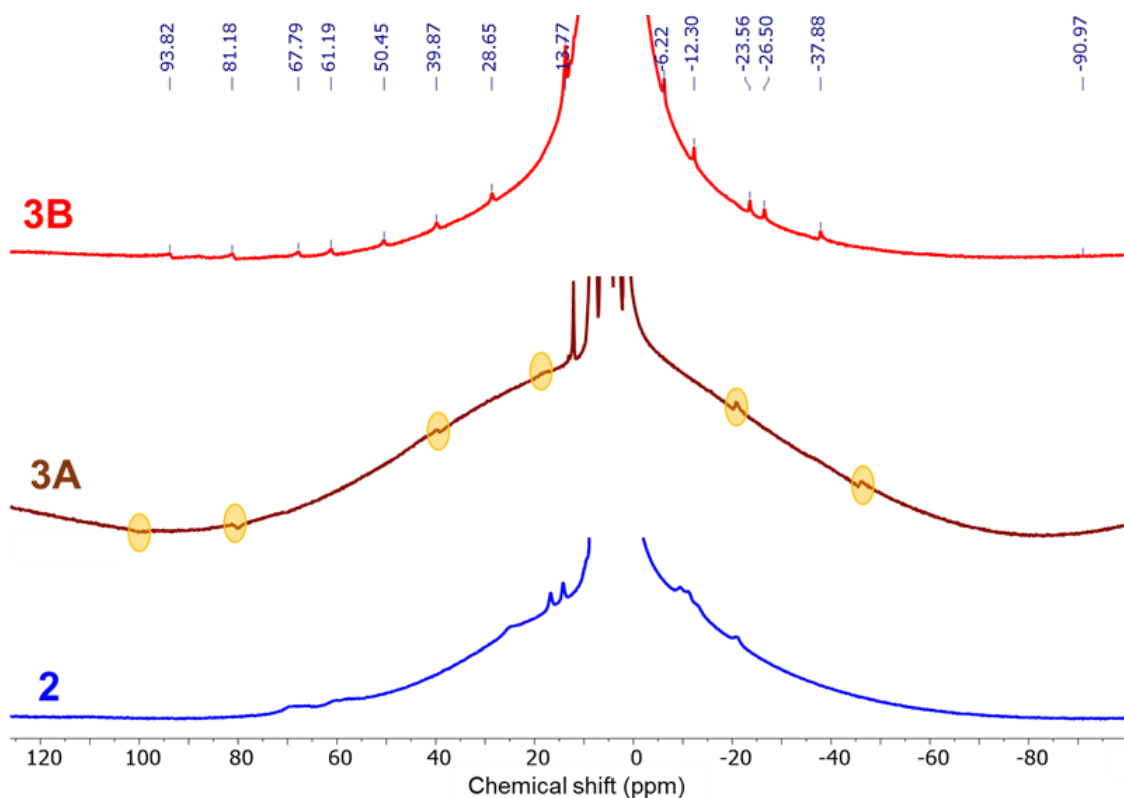
Figure S8: ^{1}H NMR (400 MHz) spectrum of **2** and **3A** and in CD$_3$OD and **3B** in CD$_3$CN at -40 °C. *Conditions to prepare 2*: 4 mM **1** + 2 eq. Et$_3$N + 10 eq. H$_2$O$_2$ at 0 °C. *Conditions to prepare 3A*: Adding 10 eq. HClO$_4$ to **2** in CD$_3$OD at -40 °C. *Conditions to prepare 3B: Addition of 10 eq. HClO$_4$ to 2 in CD$_3$CN at -40 °C.*
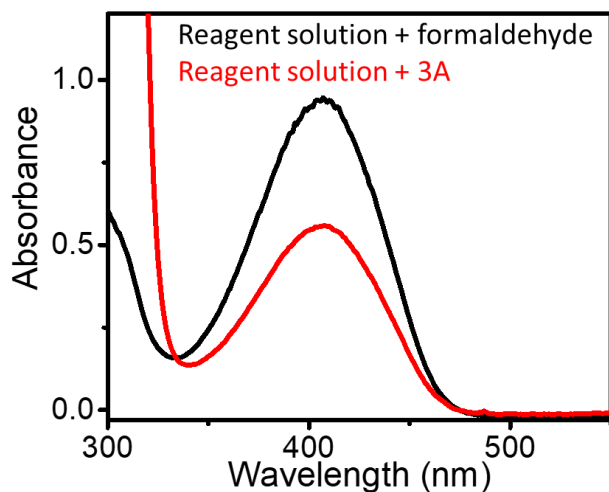
Figure S9: UV/Vis absorption spectra showing the formation of 412 nm species with the addition of reagent solution to **3A** in MeOH at 25 °C. The formation of 412 nm species indicates the presence of formaldehyde in the reaction mixture.
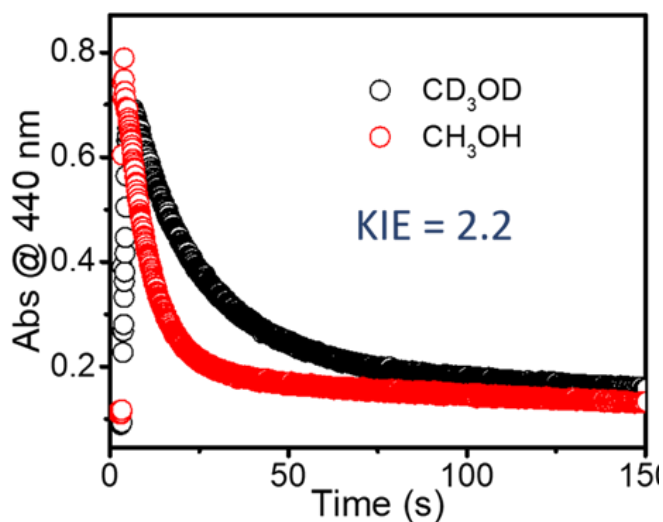
**Figure S10:** Time traces showing the decay of the 440 nm band due to **3A** in CH_3OH (red) and CD_3OD (black).
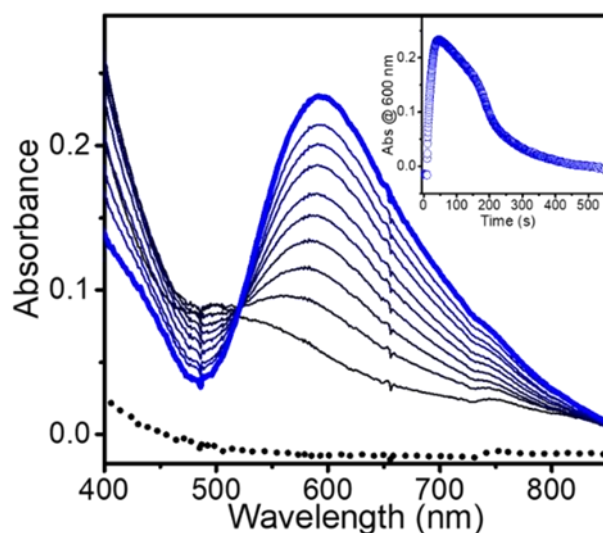
Figure S11: UV/Vis absorption spectral changes showing the formation of **2** (blue) by reaction of **1** (black) with 10 eq. of H_2O_2 and 2 eq. of Et_3N in MeCN at room temperature. The inset shows the change in absorbance at 600 nm with time.
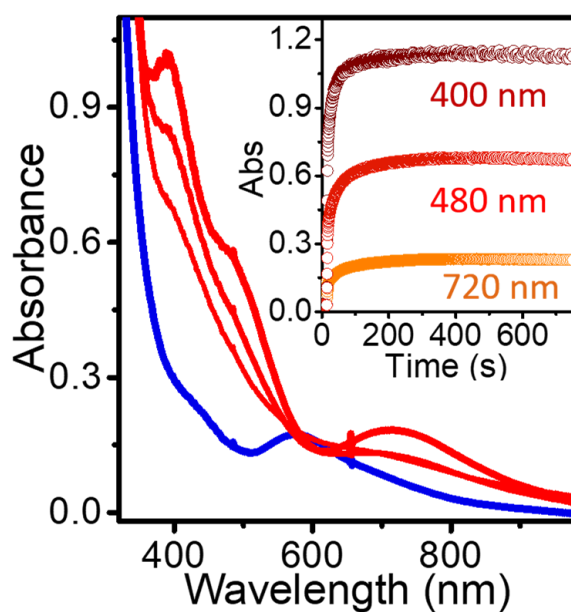

Figure S12: UV/Vis absorption spectral changes showing the formation of **3B** after adding 10 eq. of $HClO_4$ to **2** in MeCN at -40 °C. *Conditions to generate 2:* **1** + 10 eq. of H_2O_2 + 2 eq. of Et_3N in MeCN at room temperature. The inset shows the time traces of 400, 480, and 720 nm bands.
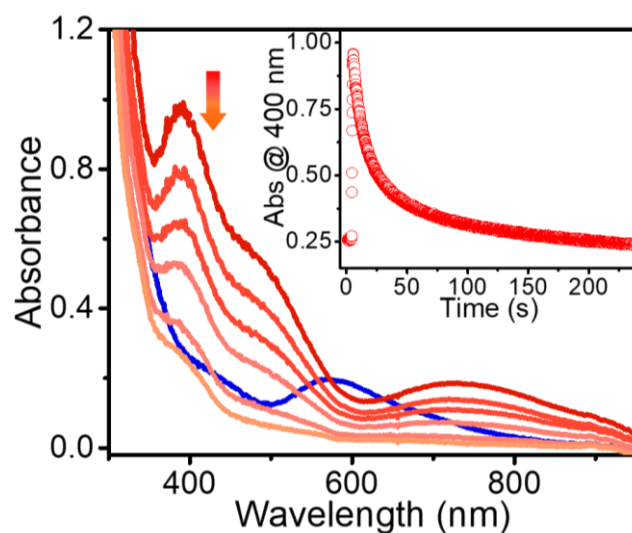
Figure S13: UV/Vis absorption spectral changes showing the formation of **3B** after adding 10 eq. of HClO$_4$ to **2** in MeCN at room temperature. *Conditions to generate 2:* **1** + 10 eq. of H$_2$O$_2$ + 2 eq. of Et$_3$N in MeCN at room temperature. The inset shows the decay of the 400 nm band with time.
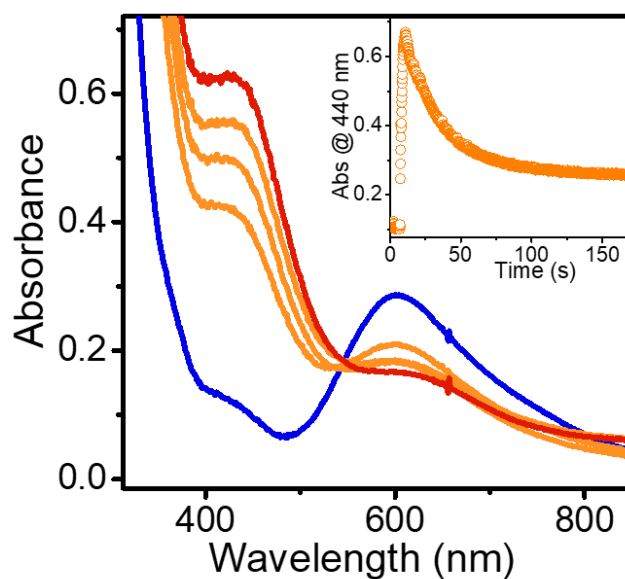
Figure S14: UV/Vis absorption spectral changes showing the formation of **3A** after adding 10 eq. of HClO$_4$ to **2** in MeCN:MeOH (1:1) at -40 °C. *Conditions to generate 2:* 1 mM **1** + 10 eq. of H$_2$O$_2$ + 2 eq. of Et$_3$N in MeCN:MeOH (1:1) at room temperature. The inset shows the decay profile of 440 nm species.
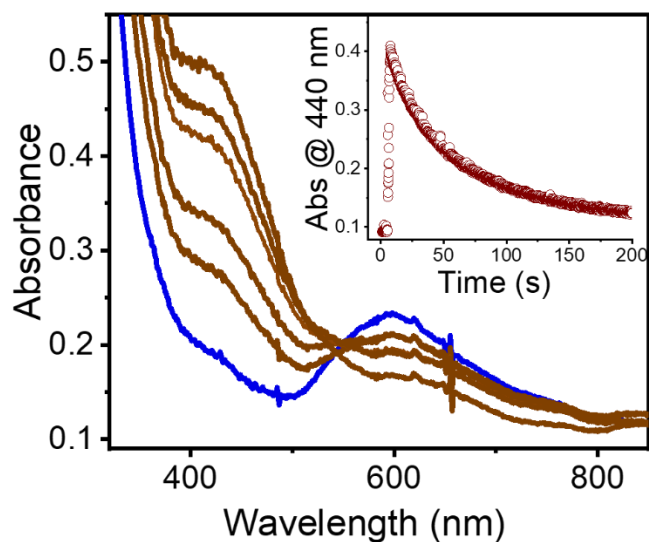
Figure S15: UV/Vis absorption spectral changes showing the formation of **3A** after adding 10 eq. of HClO$_4$ to **2** in MeCN:MeOH (9:1) at -40 °C. *Conditions to generate 2:* 1mM **1** + 10 eq. of H$_2$O$_2$ + 2 eq. of Et$_3$N in MeCN:MeOH (9:1) at room temperature. The inset shows the decay profile of 440 nm species.
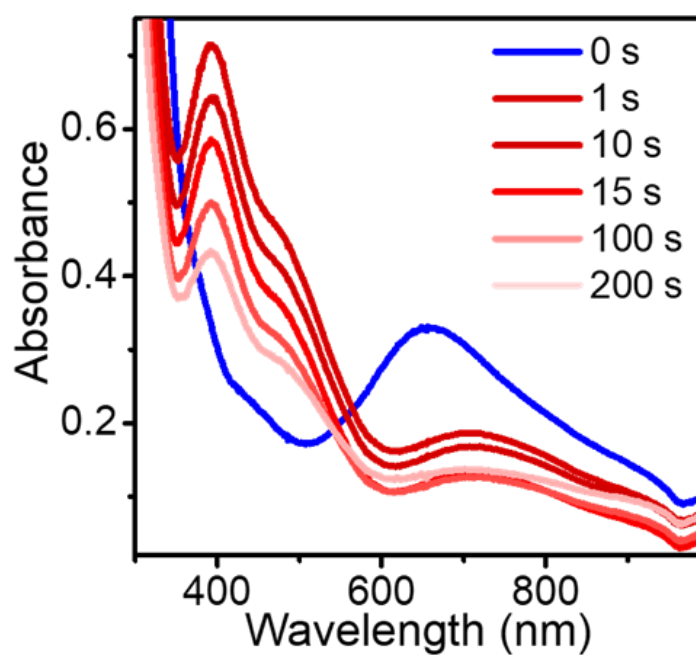
Figure S16: UV/Vis absorption spectral changes showing the formation and decay of **3B** after adding 20 eq. of HClO$_4$ to **2** (blue trace) in H$_2$O at 5 °C. *Conditions to generate 2:* 1 mM **1** + 10 eq. of H$_2$O$_2$ + 5 eq. of Et$_3$N in H$_2$O at room temperature.
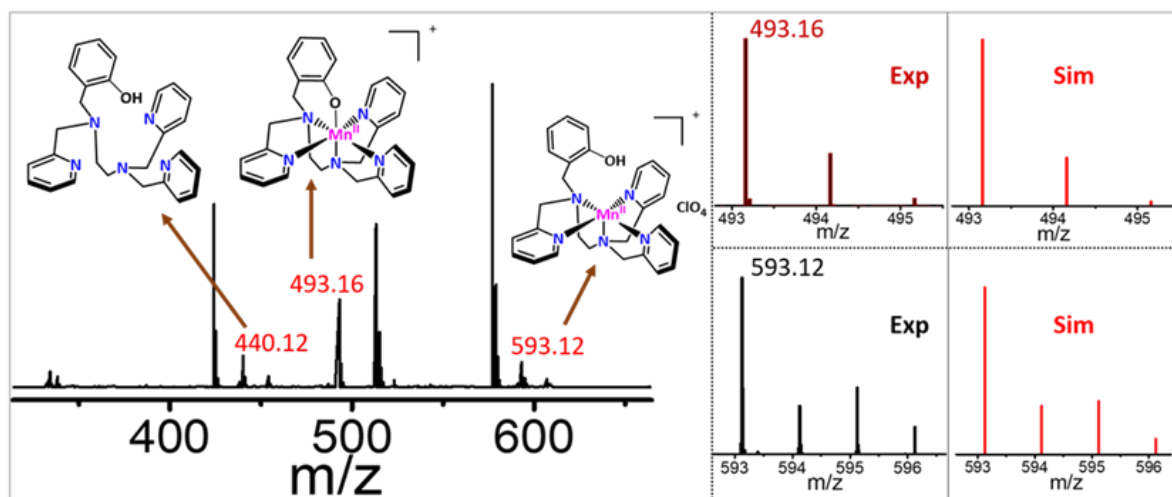
Figure S17: ESI-MS analysis of **3B** in MeCN. *Conditions to generate 3B: **2** + 10 eq. of HClO₄ in MeCN Conditions to generate **2**: **1** + 10 eq. of H₂O₂ + 2 eq. of Et₃N in MeCN.*
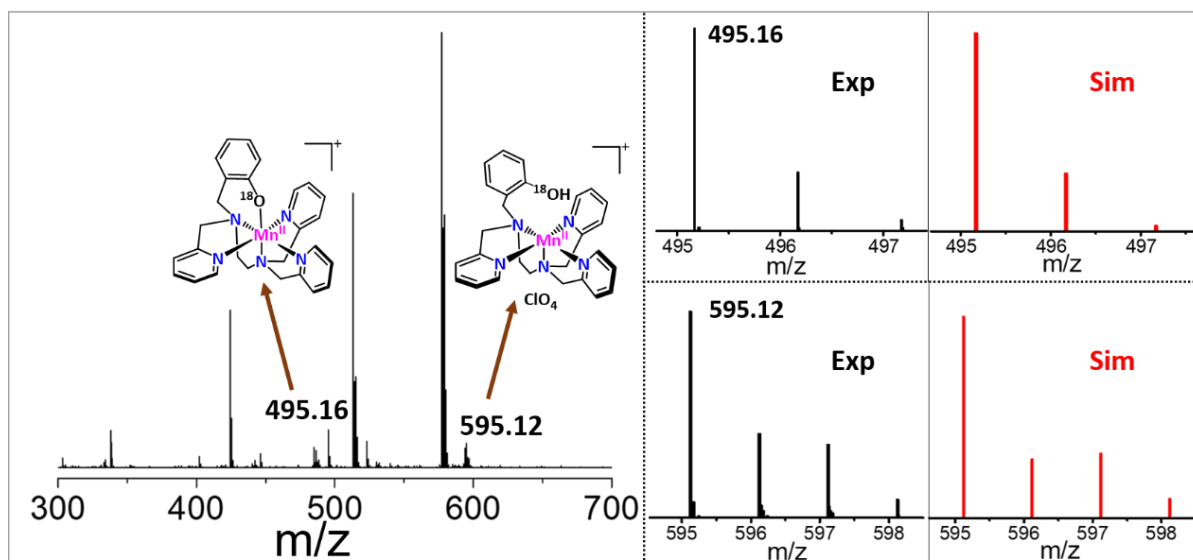
Figure S18: ESI-MS analysis of ^{18}**O-3B** in MeCN. *Conditions to generate ^{18}O-3B: **2** + 10 eq. of HClO₄ in MeCN Conditions to generate **2**: **1** + 10 eq. of H₂^{18}O₂ + 2 eq. of Et₃N in MeCN.*
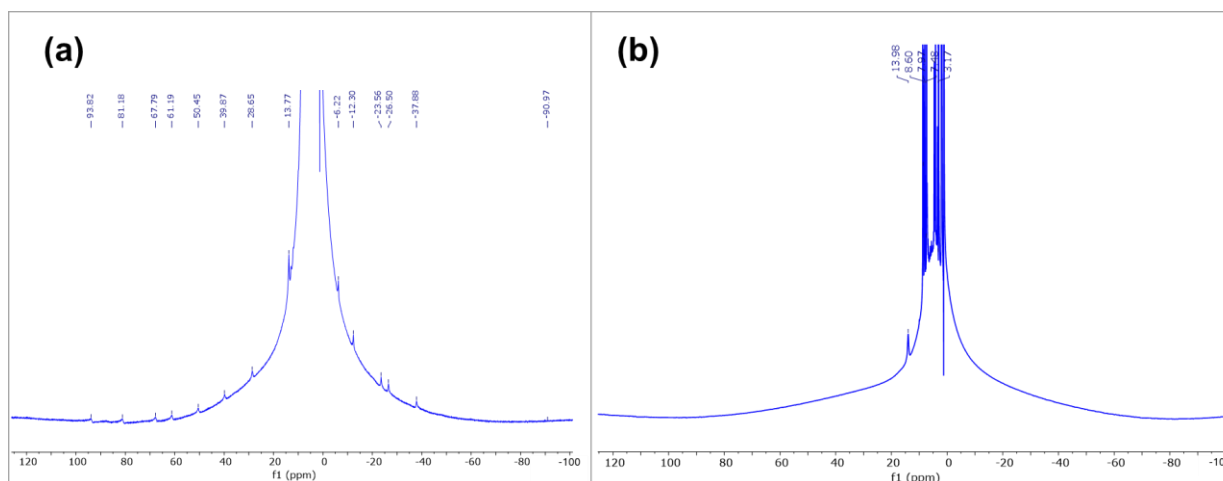
Figure S19: (a) ^{1}H NMR (400 MHz) spectra of **3B** in CD$_3$CN at -40 °C. (b) ^{1}H NMR (400 MHz) spectra of a decayed sample of **3B** in CD$_3$CN at -40 °C. *Conditions to prepare 3B*: Addition of 10 eq. HClO$_4$ to **2** in CD$_3$CN at -40 °C. *Conditions to prepare 2*: 4 mM **1** + 2 eq. Et$_3$N + 10 eq. H$_2$O$_2$ in CD$_3$CN.
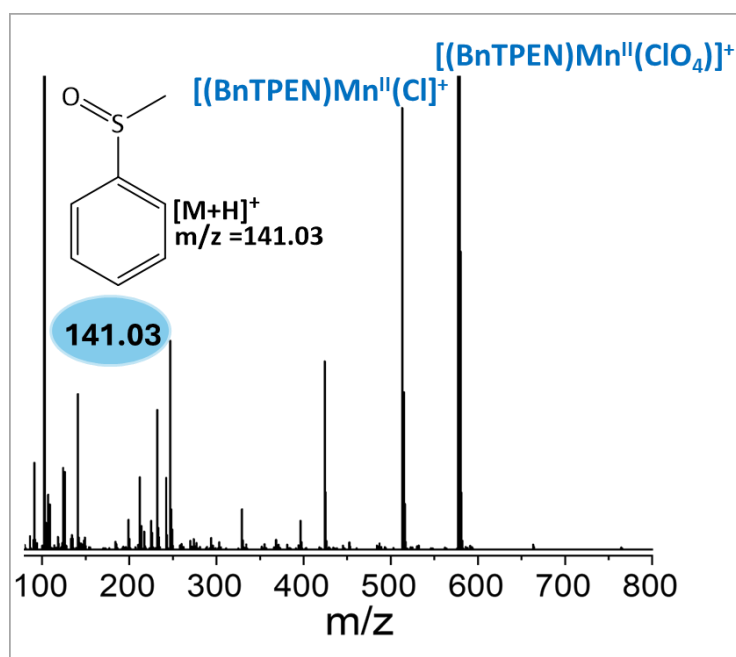
Figure S20: Product analysis of the reaction mixture of **2** + 50 eq. of thioanisole + 10 eq. of HClO$_4$ by ESI-MS. *Conditions to generate 2:* **1** + 10 eq. of H$_2$O$_2$ + 2 eq. of Et$_3$N in MeCN.
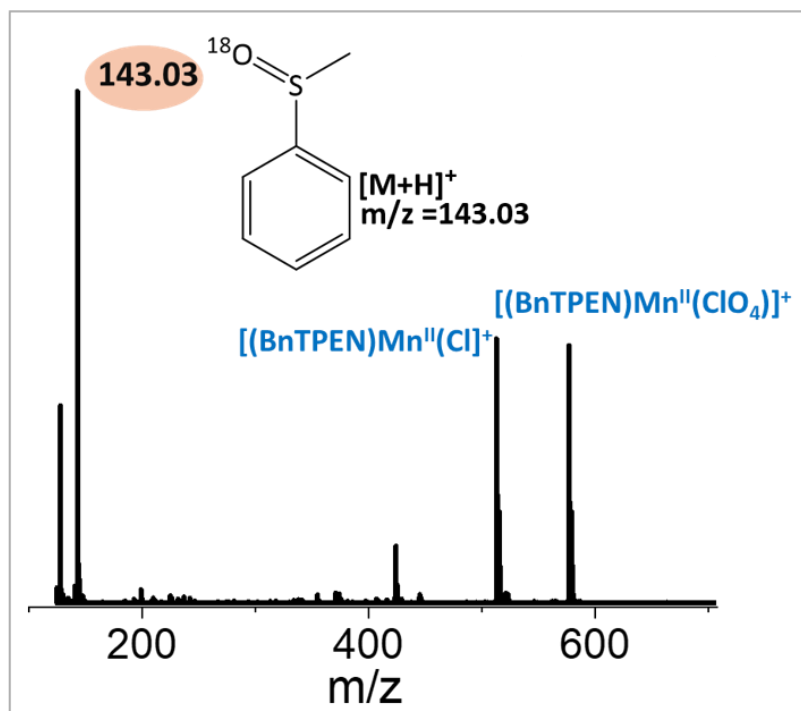
Figure S21: Product analysis of the reaction mixture of **2** + 50 eq. of thioanisole + 10 eq. of HClO$_4$ by ESI-MS. *Conditions to generate* **2***:* **1** + 10 eq. of H$_2$^{18}O$_2$ + 2 eq. of Et$_3$N in MeCN.
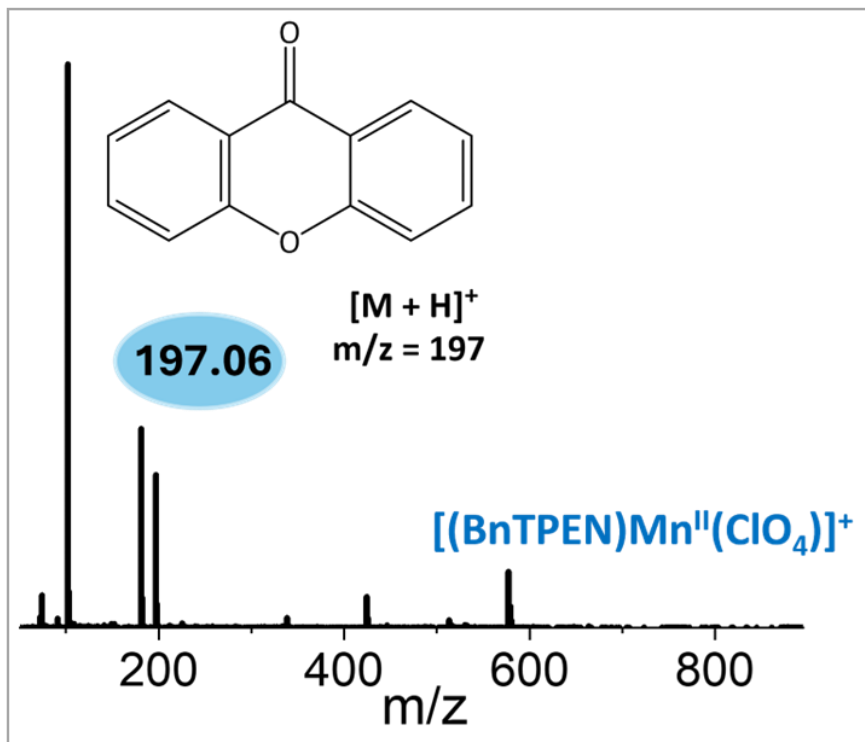
Figure S22: Product analysis of the reaction mixture of **2** + 50 eq. of xanthene + 10 eq. of HClO$_4$ by ESI-MS. *Conditions to generate* **2***:* **1** + 10 eq. of H$_2$O$_2$ + 2 eq. of Et$_3$N in MeCN.
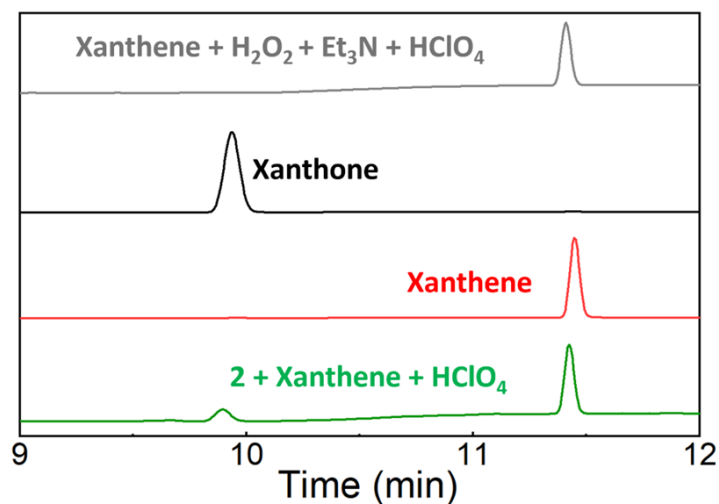
Figure S23: Product analysis of the reaction mixture of xanthene with **2** in the presence of 10 eq. HClO₄ in CH₃CN (green), H₂O₂ in the presence of eq. Et₃N and HClO₄ with 10 eq. xanthene without Mn complex under the same conditions (grey), xanthone (black), and xanthene in CH₃CN by HPLC. Note: HPLC analysis confirms that H₂O₂ in the presence of HClO₄ and Et₃N cannot convert xanthene to xanthone. This suggests that without the Mn complex, oxidants are incapable of oxidizing xanthene to xanthone.
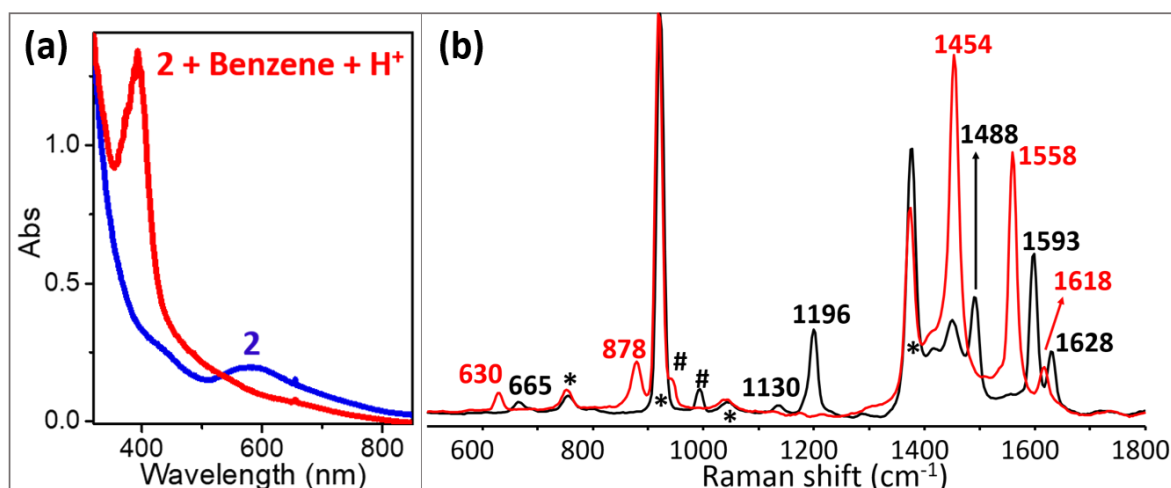
Fig. S24: (a) UV/Vis absorption spectral changes showing the formation of 390 nm species. (b) Resonance Raman spectra of 390 nm species using λ_{exc} = 405 nm in MeCN at -40 °C. * Indicate solvent peak and # indicate reagent (benzene) peak. Condition to generate 390 nm species: 1 mM **2** + 50 eq. of benzene + 10 eq. of HClO₄ in MeCN at -40 °C. Condition to generate **2**: 1 mM **1** + 10 eq. of H₂O₂ + 2 eq. of Et₃N in MeCN at room temperature.

Even lower amounts of H_2O_2 (2 eq.) can generate species **2**, albeit with a reduced yield. Using a lower concentration of H_2O_2 (2 eq.) in the presence of Et_3N and $HClO_4$ still allows for the oxidation of substrates (such as benzene) but results in a decreased yield of the substrate-oxidized product (390 nm species) (Figure S25).
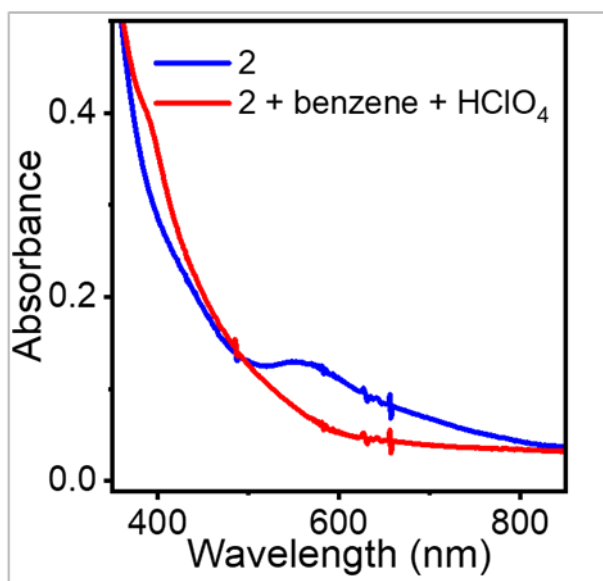
Figure S25: UV/Vis absorption spectra showing the formation of 390 nm species with low yield upon adding 10 eq. $HClO_4$ to **2** produced using 2 eq. of H_2O_2 + 2 eq. of Et_3N. Condition to generate 390 nm species: 1 mM **2** + 50 eq. of benzene + 10 eq. of $HClO_4$ in MeCN at -40 °C. *Condition to generate 2*: 1 mM **1** + 2 eq. of H_2O_2 + 2 eq. of Et_3N in MeCN at room temperature.
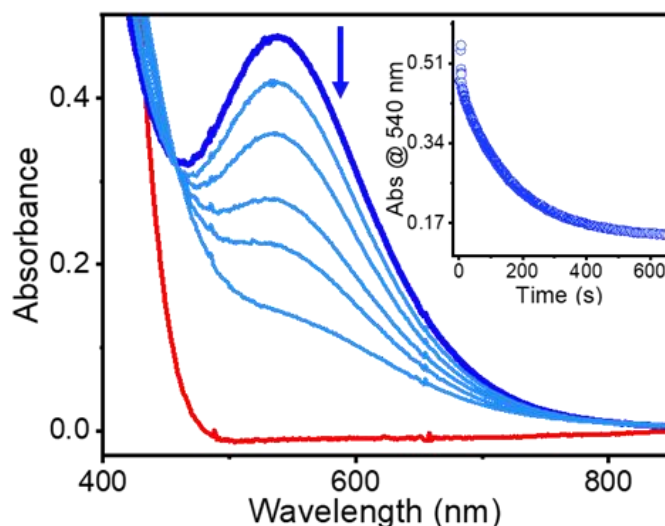
Figure S26: UV/Vis absorption spectral changes showing the decay of 540 nm band after adding 1 eq. of $HClO_4$ to $[(BnTPEN)Fe^{III}-OOH]^{2+}$ in MeOH at 0 °C. *Conditions to generate $[(BnTPEN)Fe^{III}-OOH]^{2+}$:* $(BnTPEN)Fe^{II}$ + 10 eq. of H_2O_2 in MeOH at 0 °C.
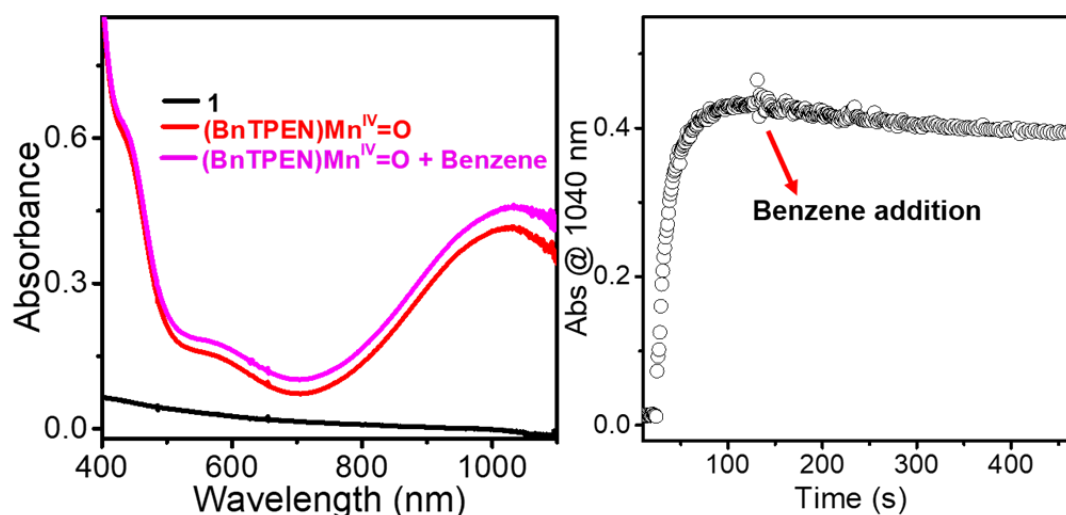
Figure S27: (left) UV/Vis absorption spectral changes showing the reaction of [(BnTPEN)Mn^{IV}=O]$^{2+}$(red) with benzene (pink). (right) The corresponding changes in absorbance at 1040 nm over time. *Condition to generate [(BnTPEN)Mn^{IV}=O]$^{2+}$:* 2 mM **1** + 2.5 eq. of PhIO in TFE at room temperature.

Nam and co-workers have reported that the addition of HOTf to [(BnTPEN)Mn^{IV}=O]$^{2+}$ (at 1020 nm) in a 1:1 mixture of TFE and MeCN resulted in the formation of a band at 580 nm, attributed to [(BnTPEN)Mn^{IV}=O•••(HOTf)$_2$]$^{2+}$.[6] Following the literature methodology, we generated 580 nm absorbing species by adding 10 eq. of HClO$_4$ to [(BnTPEN)Mn^{IV}=O]$^{2+}$ in TFE, resulting in the appearance of a band at 580 nm at room temperature. Upon the addition of benzene to the 580 nm species, there was no alteration in the decay rate of the 580 nm band (Figure S28). Furthermore, the absence of the appearance of the 390 nm band suggests that Mn^{IV}-oxo is not capable of oxidizing benzene in TFE, even in the presence of 10 eq. of HClO$_4$. It could be argued that TFE might pose challenges during the reactivity. For a more appropriate comparison, MeCN would be an ideal choice.
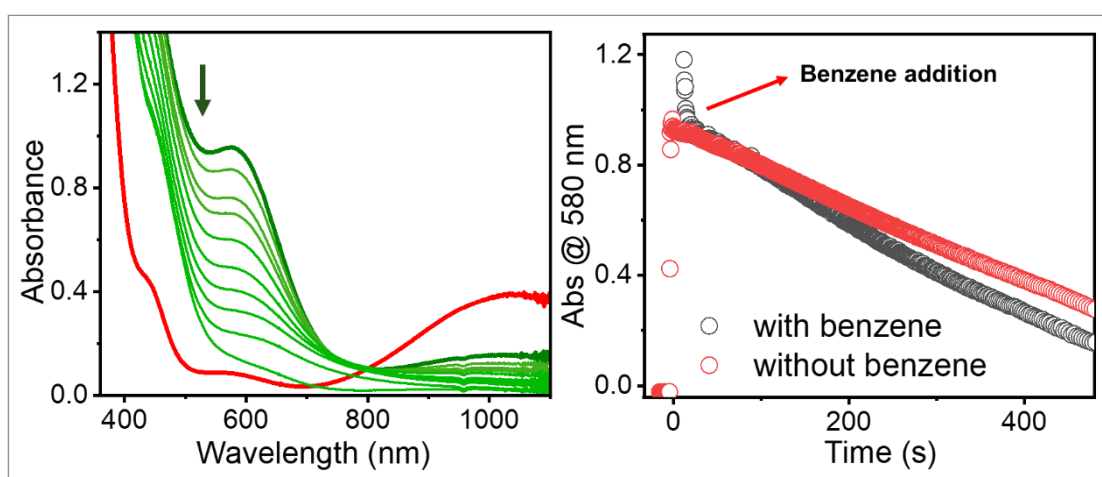
Figure S28: (a) UV-Vis spectrum depicting the formation of 580 nm band upon the addition of 10 eq. HClO$_4$ to (BnTPEN)Mn^{IV}=O (red) in TFE at RT. *Conditions to generate (BnTPEN)Mn^{IV}=O:* 1 mM **1** + 2.5 eq. PhIO in TFE at RT. (b) Time traces depicting the decay profile of 580 nm species in the presence (black) and absence (red) of 50 eq. of benzene as a substrate.

Our research group recently reported the generation of (BnTPEN)Mn[IV]-OH (which absorbs at 620 nm) by adding $HClO_4$ to (BnTPEN)Mn[III]-O-Ce[IV] in MeCN at room temperature.[5] The addition of benzene to (BnTPEN)Mn[IV]-OH in MeCN did not alter the decay profile of the 620 nm band for Mn[IV]-OH (Figure S29). This experiment also suggests that (BnTPEN)Mn[IV]-OH in the MeCN complex is not capable of oxidizing phenyl rings either intramolecularly or intermolecularly.
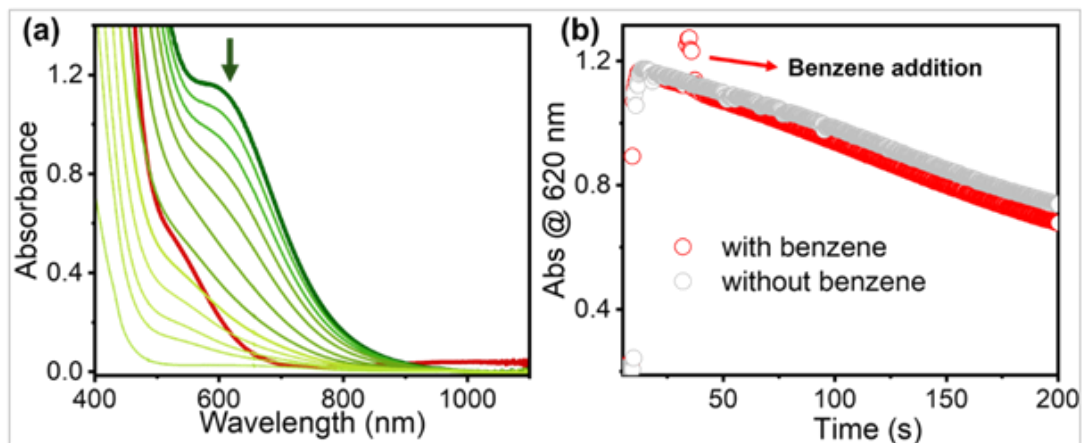
Figure S29: (a) UV-Vis spectrum depicting the formation of 620 nm band upon the addition of 10 eq. $HClO_4$ to (BnTPEN)Mn[III]-O-Ce[IV] (red) in CH_3CN at RT. Conditions to generate (BnTPEN)Mn[III]-O-Ce[IV]: 1mM **1** + 20 μl H_2O + 4 eq. CAN in CH_3CN at RT. (b) Time traces depicting the decay profile of 620 nm species in the absence (black) and presence (red) of 50 eq. of benzene as a substrate.

The potential involvement of hydroxyl radicals can be assessed using the method described by Indra and co-workers.[7] Terephthalic acid can serve as a radical trap to detect hydroxyl radicals formed in the solution. In the presence of OH[•] radicals, terephthalic acid is oxidized to 2-hydroxyterephthalic acid, which exhibits a characteristic emission peak at 439.4 nm in the fluorescence spectrum. However, our experiments showed no evidence of 2-hydroxyterephthalic acid (emission peak at 439.4 nm) in the solution of **3A** and **3B** when terephthalic acid was added (Figure S30). These findings may suggest that there is no homolysis of Mn[III]-OOH occurring in this case.
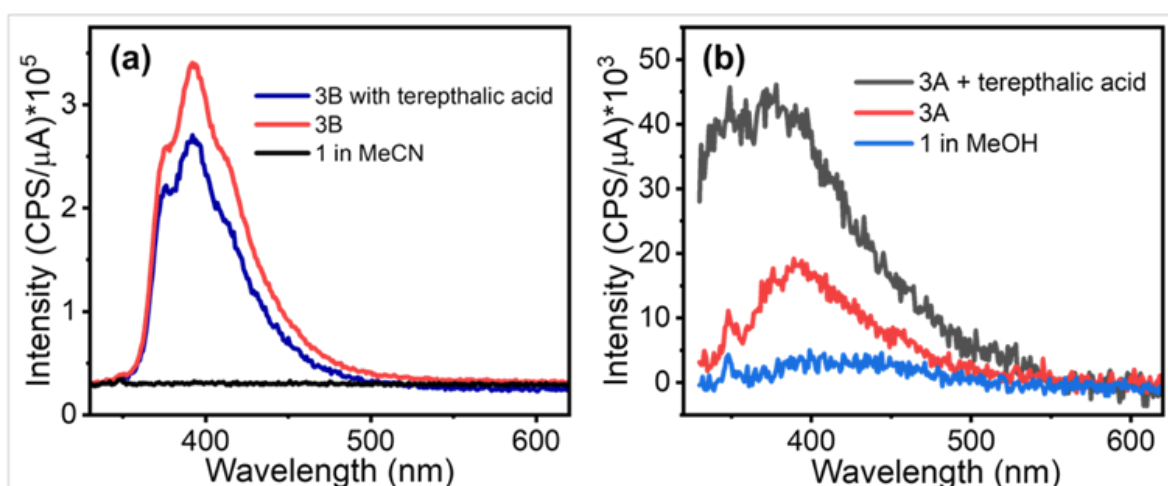
Figure S30: (a) Fluorescence spectrum of **1** in MeCN (black), **3B** (red), a mixture of terephthalic acid, and 3B (blue) in MeCN. (b) Fluorescence spectrum of **1** in MeOH (blue), **3A** (red), a mixture of terephthalic acid, and **3A** (black) in MeOH.

Computational methods:

All geometries optimizations and frequency computations were performed in Gaussian16, with B3LYP as the functional using the unrestricted formalism with Grimme's D3 empirical dispersion with Becke-Johnson correction and def2-SVP as the basis set. Solvent effects were accounted for using the polarized continuum model as implemented in Gaussian 16. Single points were computed using B3LYP functional with Grimme's D3 empirical dispersion with Becke-Johnson correction and 6-311+G(d,p) basis set. Acetonitrile was used as the solvent for all computations. Ultrafine grid was used for all computations. Stability analysis was performed to verify the stability of the wave function. XQC and YQC algorithms were used when necessary for scf convergence.

Key words used:

For optimizations:

#P B3LYP def2SVP opt freq=noraman scrf=(pcm,solvent-acetonitrile) empiricaldispersion=gd3bj

For stability analysis,

Stable = opt

For single points: #P UB3LYP gfinput IOP(6/7=3) 6-311+G(d,p) empiricaldispersion=gd3bj

For TS search: #p opt=(calcfc,ts,noeigen,nofreeze) freq=noraman ub3lyp scrf=(solvent=acetonitrile,pcm) def2svp empiricaldispersion=gd3bj

Transition state search for the oxidation of the pendant benzyl group of the ligand by the putative Mn(V)=O oxo species. Two mechanistic pathways were conceived for this process viz., (I) the direct hydrogen atom abstraction by Mn(V)=O (TS_{HAT}) and (II) $S_{RN}1$ type attack of Mn(V)=O species on the benzyl group (TS_{SRN1}) followed by hydrogen atom abstraction. Investigating these two pathways using computations revealed that TS_{SRN1} is the favored pathway by 10.9 kcal/mol compared to TS_{HAT}. These TSS energies are reported with respect to each other ($\Delta\Delta G^{\ddagger}$) to compare them with each other. Further details related to the energy profile are currently underway along with a more rigorous computational treatment for the system.

(A) (B) (C)

TS_{HAT} (10.9 kcal/mol) TS_{SRN1} (0.0 kcal/mol) TS_{HT} (3.2 kcal/mol)
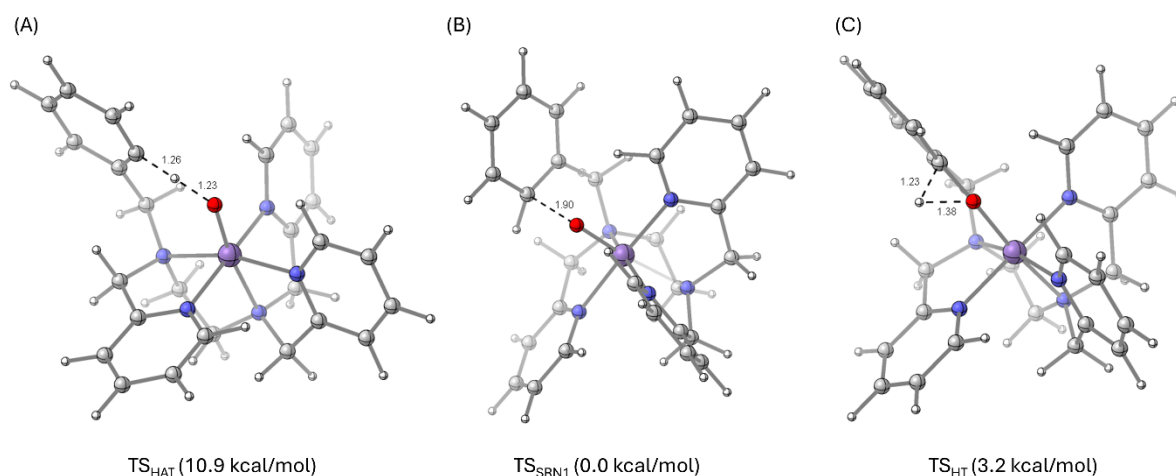
Figure S31: TS for the oxidation of the phenyl group on the triplet surface computed at UB3LYP-D3BJ/6-311+G(d,p)//PCM(CH$_3$CN)-UB3LYP-D3BJ/def2-SVP level of theory.

Deuterium kinetic isotope effects were predicted using Mayer-Bigeleisen equations[8] as implemented in isoeff. The following input file was used for computing the deuterium isotope effects

```
$GLOBAL MEMORY=2000000 $END
 $IODEF SSINP = Methanol.log TSINP = kie_OSS_HAT_Oxo_G2.log $END

---------1-2H-------
 $ISOEFF HMASS(2) = 2 HMATS(65) = 2 KIE= .T. EIE= .F. $END
 $ISOEFF HMASS(3) = 2 HMATS(66) = 2 KIE= .T. EIE= .F. $END
 $ISOEFF HMASS(4) = 2 HMATS(67) = 2 KIE= .T. EIE= .F. $END
 $ISOEFF HMASS(6) = 2 HMATS(69) = 2 KIE= .T. EIE= .F. $END
 $ISOEFF SCFACT=0.9614 $END
 $ISOEFF TKELV(1) = 298 $END

-$-
```

Key portions of output from isoeff:

```
 SSFACT =  0.9614
 TSFACT =  0.9614

 ISOTOPE EFFECT(298.00) =    2.587711
```

Table S1: Table with the raw energies for the key transition states reported in the manuscript.

File	Free Energy Correction (Hartree)	Single Point (Hartree)	SP+G (Hartree)
TS$_{Methanol}$	0.522834	-2661.686143	-2661.163309
TS$_{HAT}$	0.465763	-2545.913625	-2545.447862
TS$_{SRN1}$	0.473876	-2545.93911	-2545.465234
TS$_{HT}$	0.470724	-2545.930808	-2545.460084

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XYZ Coordinates:

```
69
TS_Methanol
69
Final Energy =           -2661.6861432900
C        -3.3161500      -0.0766000      -0.9059820
C        -3.4033560      -0.1969400       1.4403190
C        -4.7911530      -0.2621910       1.4157920
C        -5.4493030      -0.2293950       0.1850220
C        -4.7012950      -0.1416480      -0.9916290
H        -2.8396850      -0.2158390       2.3728070
H        -5.3394470      -0.3390640       2.3547530
H        -6.5382820      -0.2817710       0.1385730
H        -5.1804780      -0.1296710      -1.9707940
C        -2.3924920       0.0376290      -2.0835630
H        -2.1907350       1.0936320      -2.3094590
H        -2.8257740      -0.4073560      -2.9906960
N        -1.1187690      -0.6284620      -1.7084880
C         0.0437810      -0.1774980      -2.5208680
H         0.0364540      -0.6552310      -3.5121020
H        -0.0419660       0.9033680      -2.6841470
C         1.3016190      -0.5366230      -1.7663490
H         1.3866820      -1.6251570      -1.6633150
H         2.1961690      -0.1893640      -2.2997240
N         1.2742170       0.0454350      -0.3812710
C        -1.2945340      -2.1114270      -1.7611120
H        -0.7876410      -2.5242960      -2.6449640
H        -2.3626190      -2.3395940      -1.8907720
C        -0.8388190      -2.7884050      -0.5067840
C        -0.7158130      -4.1746680      -0.4230960
C        -0.3928120      -4.7542040       0.8012220
H        -0.8833850      -4.7832320      -1.3120270
C        -0.3241660      -2.5589110       1.7621610
C        -0.2059960      -3.9309760       1.9157480
H        -0.2928130      -5.8374120       0.8875070
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H        -0.1718950        -1.8730330         2.5953930
H         0.0375540        -4.3417770         2.8955810
C         1.6650580         1.4851050        -0.3903860
H         2.4761960         1.6623410        -1.1083630
H         2.0514120         1.7456360         0.6060020
C         2.2085920        -0.7317490         0.5374560
H         1.9104250        -1.7820470         0.4710560
H         2.0098100        -0.3798580         1.5561370
C         0.5042880         2.3929780        -0.6230610
C         0.6617330         3.7077470        -1.0536150
C        -1.7846900         2.7329290        -0.2611180
C        -0.4480850         4.5491800        -1.0792000
H         1.6490720         4.0613260        -1.3507360
C        -1.6884090         4.0559620        -0.6607350
H        -2.7329980         2.3191190         0.0739370
H        -0.3471200         5.5831190        -1.4130460
H        -2.5779070         4.6853870        -0.6444090
C         3.6693820        -0.5792910         0.1967390
C         4.2710770        -1.3949480        -0.7755570
C         4.4547190         0.3756730         0.8618470
C         5.6209280        -1.2383650        -1.0956700
H         3.6890450        -2.1709580        -1.2766530
C         5.8052390         0.5317950         0.5440190
H         4.0144310         0.9922110         1.6485470
C         6.3888710        -0.2701770        -0.4411490
H         6.0761840        -1.8807110        -1.8523220
H         6.4039310         1.2764580         1.0726420
H         7.4454390        -0.1494800        -0.6901940
N        -2.6945320        -0.0983040         0.2989110
N        -0.6227900        -2.0035930         0.5663550
N        -0.7081530         1.9138180        -0.2591020
Mn       -0.6939530        -0.0027070         0.2967610
O        -0.4513160         0.2165030         1.8507430
C         0.1068070         2.5972550         2.8889140
H        -0.1950200         1.5293480         2.4432670
H        -0.6483220         3.2747500         2.4662240
H        -0.0098650         2.4300070         3.9719910
O         1.3594150         2.9500860         2.4829550
H         2.0272240         2.6084340         3.0996860
OSS_HAT_Oxo_G1.log
69
Final Energy =          -2661.6782409500
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C         3.3518350         0.4648700         1.1337360
C         4.7159520         0.6953870         1.0071780
C         5.2727940         0.7849940        -0.2699000
C         4.4486240         0.6446190        -1.3889280
H         2.8693270         0.3883910         2.1072740
H         5.3241200         0.8065380         1.9049400
H         6.3403800         0.9723840        -0.3957160
H         4.8464770         0.7234600        -2.4007670
C         2.0992560         0.2119890        -2.3109650
H         2.0046750        -0.8556160        -2.5545530
H         2.4082040         0.7228250        -3.2339670
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N	0.7900590	0.7169940	-1.8235050
C	-0.3745670	0.1489200	-2.5541240
H	-0.4966350	0.6344010	-3.5339350
H	-0.1885310	-0.9151330	-2.7419000
C	-1.5981460	0.3665610	-1.6963840
H	-1.7850710	1.4394100	-1.5674990
H	-2.4938480	-0.0666390	-2.1605130
N	-1.3970660	-0.2215130	-0.3287770
C	0.7835980	2.2113040	-1.8522740
H	0.1195800	2.5723070	-2.6506550
H	1.7906160	2.5678750	-2.1129620
C	0.4112820	2.8132170	-0.5331400
C	0.1839020	4.1817830	-0.3903880
C	-0.0697700	4.6990650	0.8771020
H	0.2163900	4.8254010	-1.2700030
C	0.1325660	2.4815020	1.7650020
C	-0.0854120	3.8332820	1.9749450
H	-0.2497610	5.7671690	1.0093120
H	0.1152940	1.7647210	2.5859350
H	-0.2717650	4.1948640	2.9862400
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H	-2.4847810	-1.9475540	-0.9771580
H	-1.9186780	-1.9865410	0.6950960
C	-2.3265160	0.4456460	0.6768290
H	-2.1059790	1.5161670	0.6465980
H	-2.0409660	0.0612080	1.6631190
C	-0.4140640	-2.4760260	-0.6815500
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C	0.7148790	-4.5031310	-1.2982310
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C	1.9287480	-3.8919750	-0.9701340
H	2.8475150	-2.0691110	-0.2724850
H	0.6930950	-5.5313800	-1.6628290
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Mn	0.6024330	0.0097170	0.2021090
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C	1.0272320	-2.6039360	3.0423210
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H	0.0430830	-3.0522630	3.2461240

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H        1.6746360      -3.2627490       2.4398040
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OSS_HAT_Oxo_G2.log
69
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C       -3.3161500      -0.0766000      -0.9059820
C       -3.4033560      -0.1969400       1.4403190
C       -4.7911530      -0.2621910       1.4157920
C       -5.4493030      -0.2293950       0.1850220
C       -4.7012950      -0.1416480      -0.9916290
H       -2.8396850      -0.2158390       2.3728070
H       -5.3394470      -0.3390640       2.3547530
H       -6.5382820      -0.2817710       0.1385730
H       -5.1804780      -0.1296710      -1.9707940
C       -2.3924920       0.0376290      -2.0835630
H       -2.1907350       1.0936320      -2.3094590
H       -2.8257740      -0.4073560      -2.9906960
N       -1.1187690      -0.6284620      -1.7084880
C        0.0437810      -0.1774980      -2.5208680
H        0.0364540      -0.6552310      -3.5121020
H       -0.0419660       0.9033680      -2.6841470
C        1.3016190      -0.5366230      -1.7663490
H        1.3866820      -1.6251570      -1.6633150
H        2.1961690      -0.1893640      -2.2997240
N        1.2742170       0.0454350      -0.3812710
C       -1.2945340      -2.1114270      -1.7611120
H       -0.7876410      -2.5242960      -2.6449640
H       -2.3626190      -2.3395940      -1.8907720
C       -0.8388190      -2.7884050      -0.5067840
C       -0.7158130      -4.1746680      -0.4230960
C       -0.3928120      -4.7542040       0.8012220
H       -0.8833850      -4.7832320      -1.3120270
C       -0.3241660      -2.5589110       1.7621610
C       -0.2059960      -3.9309760       1.9157480
H       -0.2928130      -5.8374120       0.8875070
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H        2.4761960       1.6623410      -1.1083630
H        2.0514120       1.7456360       0.6060020
C        2.2085920      -0.7317490       0.5374560
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H        2.0098100      -0.3798580       1.5561370
C        0.5042880       2.3929780      -0.6230610
C        0.6617330       3.7077470      -1.0536150
C       -1.7846900       2.7329290      -0.2611180
C       -0.4480850       4.5491800      -1.0792000
H        1.6490720       4.0613260      -1.3507360
C       -1.6884090       4.0559620      -0.6607350
H       -2.7329980       2.3191190       0.0739370
H       -0.3471200       5.5831190      -1.4130460
H       -2.5779070       4.6853870      -0.6444090
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C      3.6693820     -0.5792910      0.1967390
C      4.2710770     -1.3949480     -0.7755570
C      4.4547190      0.3756730      0.8618470
C      5.6209280     -1.2383650     -1.0956700
H      3.6890450     -2.1709580     -1.2766530
C      5.8052390      0.5317950      0.5440190
H      4.0144310      0.9922110      1.6485470
C      6.3888710     -0.2701770     -0.4411490
H      6.0761840     -1.8807110     -1.8523220
H      6.4039310      1.2764580      1.0726420
H      7.4454390     -0.1494800     -0.6901940
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N     -0.7081530      1.9138180     -0.2591020
Mn    -0.6939530     -0.0027070      0.2967610
O     -0.4513160      0.2165030      1.8507430
C      0.1068070      2.5972550      2.8889140
H     -0.1950200      1.5293480      2.4432670
H     -0.6483220      3.2747500      2.4662240
H     -0.0098650      2.4300070      3.9719910
O      1.3594150      2.9500860      2.4829550
H      2.0272240      2.6084340      3.0996860
63
OSS_TS_MnBnTPEN_Oxo_G2.log
63
Final Energy =        -2545.9134789800
C     -2.7017230     -1.2408070      0.4814260
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C     -2.3577420     -1.8626670      3.1467200
C     -3.5605800     -2.1855270      2.5156940
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H     -2.1844070     -2.0964730      4.1972310
H     -4.3585960     -2.6844590      3.0681200
H     -4.6519840     -2.1313320      0.6365310
C     -2.7646760     -0.8480740     -0.9732430
H     -3.1327330      0.1819410     -1.0789630
H     -3.4510240     -1.4958520     -1.5376270
N     -1.3802260     -0.9264840     -1.5036450
C     -1.1279200     -0.1483420     -2.7448930
H     -1.4718550     -0.6969190     -3.6341040
H     -1.7078910      0.7822510     -2.6978150
C      0.3623300      0.1238750     -2.8305370
H      0.9317640     -0.8130360     -2.8541180
H      0.6159780      0.6794690     -3.7444940
N      0.7961550      0.9084550     -1.6202750
C     -0.9918090     -2.3583780     -1.6700280
H     -1.0352600     -2.6452550     -2.7303490
H     -1.7299510     -2.9885800     -1.1526670
C      0.3480080     -2.6545050     -1.0748800
C      1.0284530     -3.8439200     -1.3299260
C      2.2161460     -4.1032900     -0.6497640
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C      1.9633920     -2.0022630      0.4777210
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C      2.6829810      -3.1711550       0.2812600
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H      3.5967700      -3.3401050       0.8511310
C      0.3420100       2.3297470      -1.7776950
H      0.1445110       2.5379820      -2.8392720
H      1.1596100       3.0081200      -1.5004460
C      2.2773140       0.8496460      -1.4649640
H      2.7316380       1.5105030      -2.2257040
H      2.6070630      -0.1660270      -1.7152310
C     -0.8592750       2.6486140      -0.9442130
C     -1.4968920       3.8847580      -1.0338960
C     -2.2713090       1.9915170       0.7966870
C     -2.5554080       4.1652550      -0.1742890
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C     -2.9401890       3.2043800       0.7654640
H     -2.5414830       1.2256550       1.5193680
H     -3.0683540       5.1269060      -0.2283360
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C      2.8204980       1.2128070      -0.1090830
C      2.0684210       1.9566850       0.8705710
C      4.0765260       0.7275260       0.2470630
C      2.6272040       2.2034100       2.1631980
H      1.2496470       2.6083900       0.5767890
C      4.5942890       0.9693310       1.5226980
H      4.6511660       0.1310560      -0.4636630
C      3.8664170       1.7023550       2.4888530
H      2.0486320       2.7928820       2.8755270
H      5.5751880       0.5661560       1.7824910
H      4.2968410       1.8757840       3.4758940
N     -1.5439530      -0.9236170       1.1142590
N      0.8303190      -1.7420950      -0.2084490
N     -1.2617900       1.7109220      -0.0589000
Mn     -0.1839460       0.0131780      -0.0136050
O      0.8214670       0.4515900       1.1870370
63
OSS_TS_MnBnTPEN_Oxo_G3.log
63
Final Energy =        -2545.9115383500
C     -3.0517100       0.1167250       0.3956680
C     -1.9336540      -0.4338210       2.3808470
C     -3.1378680      -0.5252360       3.0726450
C     -4.3295150      -0.2841180       2.3867060
C     -4.2875080       0.0373690       1.0271790
H     -0.9708450      -0.6061090       2.8653220
H     -3.1327190      -0.7826380       4.1319020
H     -5.2883930      -0.3512570       2.9034500
H     -5.1996720       0.2233620       0.4597020
C     -2.8538790       0.4921290      -1.0496050
H     -2.7004970       1.5762440      -1.1431800
H     -3.7244080       0.2317460      -1.6680190
N     -1.6263960      -0.2065830      -1.5275960
C     -1.0098550       0.3989590      -2.7441240
H     -1.5524250       0.0892470      -3.6488650
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H      -1.0967460      1.4904270     -2.6716310
C       0.4392820     -0.0434160     -2.8020520
H       0.5100170     -1.1361410     -2.8810460
H       0.9468170      0.3783260     -3.6815470
N       1.1434580      0.3737790     -1.5448900
C      -1.9323770     -1.6620200     -1.7341980
H      -2.0064790     -1.8770210     -2.8093910
H      -2.9242460     -1.8736920     -1.3096100
C      -0.9469040     -2.5656170     -1.0600540
C      -0.9203380     -3.9395600     -1.2932850
C      -0.0519370     -4.7346180     -0.5480970
H      -1.5822330     -4.3729060     -2.0437170
C       0.6897100     -2.7590790      0.5896630
C       0.7571510     -4.1345790      0.4204870
H      -0.0131180     -5.8124900     -0.7140530
H       1.2964610     -2.2544650      1.3399120
H       1.4373840     -4.7190710      1.0398370
C       1.4925660      1.8244910     -1.5911520
H       1.6417530      2.1503540     -2.6305920
H       2.4601260      1.9681870     -1.0871340
C       2.3804170     -0.4344300     -1.3600610
H       3.0577410     -0.2596030     -2.2096230
H       2.0974410     -1.4958880     -1.3964640
C       0.4867840      2.6799060     -0.8837390
C       0.4701150      4.0654530     -1.0325220
C      -1.1584460      2.7838870      0.7659100
C      -0.3957630      4.8199250     -0.2440410
H       1.1391560      4.5393090     -1.7513590
C      -1.2115810      4.1671940      0.6841340
H      -1.7848470      2.2437520      1.4721300
H      -0.4273730      5.9060870     -0.3449340
H      -1.8891140      4.7178760      1.3365640
C       3.1223640     -0.1637670     -0.0758480
C       2.4750950     -0.0074110      1.1935380
C       4.5117100     -0.1358100     -0.0784150
C       3.2225850      0.0200460      2.4052880
H       1.9275570      1.0742380      1.4104450
C       5.2507910     -0.0321910      1.1116870
H       5.0389540     -0.2146330     -1.0308370
C       4.6111850      0.0413060      2.3499720
H       2.6762110      0.0784690      3.3477160
H       6.3407840     -0.0186250      1.0608680
H       5.1881330      0.1036370      3.2733770
N      -1.9041640     -0.1173400      1.0764050
N      -0.1336360     -1.9904010     -0.1526750
N      -0.3396050      2.0501770     -0.0196540
Mn     -0.2398530      0.0212370     -0.0352250
O       1.0528490      0.0193270      1.3401370
69
Singlet_HAT_Oxo_G1.log
69
Final Energy =        -2661.6771244100
C       3.1914190      0.3007750     -1.0967160
C       3.3767850      0.4616020      1.2356500
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C     4.7517490      0.6418240      1.1441670
C     5.3544580      0.6458040     -0.1149440
C     4.5609220      0.4818500     -1.2517910
H     2.8633300      0.4557800      2.1963200
H     5.3328300      0.7804730      2.0560620
H     6.4317600      0.7890400     -0.2128440
H     4.9896630      0.5022560     -2.2539280
C     2.2194450      0.1144430     -2.2217340
H     2.0923500     -0.9541450     -2.4444230
H     2.5618020      0.5985170     -3.1477360
N     0.9215700      0.6730530     -1.7658410
C    -0.2306630      0.1551680     -2.5496070
H    -0.2956170      0.6537300     -3.5282950
H    -0.0749640     -0.9133070     -2.7421750
C    -1.4726050      0.4008460     -1.7328410
H    -1.6273890      1.4760440     -1.5825440
H    -2.3689440      0.0094250     -2.2312980
N    -1.3204040     -0.2308040     -0.3813160
C     0.9785380      2.1669730     -1.7913420
H     0.3968830      2.5519910     -2.6410920
H     2.0177280      2.4782440     -1.9713600
C     0.5335950      2.7952140     -0.5049160
C     0.3183530      4.1702380     -0.4035850
C     0.0078140      4.7182320      0.8381540
H     0.4050050      4.7956990     -1.2926340
C     0.1335280      2.5155210      1.7755400
C    -0.0740110      3.8755620      1.9501960
H    -0.1637050      5.7911880      0.9392120
H     0.0644930      1.8165950      2.6092770
H    -0.3043680      4.2607070      2.9436140
C    -1.5754740     -1.7007900     -0.4412490
H    -2.3567670     -1.9288030     -1.1779300
H    -1.9638890     -2.0157820      0.5376680
C    -2.2831720      0.4147380      0.6083780
H    -2.0182520      1.4741770      0.6579520
H    -2.0747680     -0.0393560      1.5838460
C    -0.3323070     -2.4937380     -0.6926090
C    -0.3677300     -3.7974780     -1.1805690
C     1.9740420     -2.6326450     -0.3363800
C     0.8168270     -4.5308060     -1.2351590
H    -1.3165940     -4.2286390     -1.5010240
C     2.0040850     -3.9429150     -0.7893300
H     2.8793460     -2.1415640      0.0142570
H     0.8131340     -5.5538280     -1.6149090
H     2.9489300     -4.4861130     -0.7962670
C    -3.7363350      0.2577140      0.2377640
C    -4.3735370      1.2180510     -0.5651730
C    -4.4796740     -0.8405290      0.7000020
C    -5.7150640      1.0691320     -0.9212770
H    -3.8227010      2.0978530     -0.9049750
C    -5.8216240     -0.9903240      0.3450340
H    -4.0145980     -1.5791470      1.3567490
C    -6.4398310     -0.0392580     -0.4723400
H    -6.1974940      1.8248660     -1.5446220
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H        -6.3875440       -1.8480060        0.7146120
H        -7.4898560       -0.1555560       -0.7495960
N         2.6246160        0.2819910        0.1316180
N         0.4191060        1.9888050        0.5657840
N         0.8277320       -1.9175530       -0.3034680
Mn        0.6457850       -0.0078200        0.2618200
O         0.4862300       -0.2674660        1.8151410
C         0.6378460       -2.4792660        3.1357830
H         0.6214740       -1.4677040        2.3848250
H         0.2933660       -3.2767530        2.4594320
H         1.7100970       -2.4870120        3.3802850
O        -0.1228090       -2.2219330        4.2056270
H        -1.0493710       -2.4742630        4.0498190
69
Singlet_HAT_Oxo_G2.log
69
Final Energy =          -2661.6807260300
C        -3.1555460       -0.3942470       -1.0777590
C        -3.3645550       -0.5391620        1.2534100
C        -4.7354840       -0.7412570        1.1481710
C        -5.3234700       -0.7681900       -0.1176130
C        -4.5199570       -0.6003580       -1.2467220
H        -2.8622030       -0.5164860        2.2194230
H        -5.3248080       -0.8794010        2.0548130
H        -6.3970270       -0.9304200       -0.2263670
H        -4.9373850       -0.6344440       -2.2531990
C        -2.1763800       -0.1880230       -2.1925930
H        -2.0677120        0.8837800       -2.4096020
H        -2.5005110       -0.6747220       -3.1237140
N        -0.8717000       -0.7221530       -1.7265860
C         0.2765380       -0.1741730       -2.4965910
H         0.3594900       -0.6641640       -3.4782250
H         0.1009920        0.8925280       -2.6819090
C         1.5154380       -0.4018570       -1.6703330
H         1.6878130       -1.4750660       -1.5250410
H         2.4094210        0.0088300       -2.1575910
N         1.3385570        0.2178550       -0.3166750
C        -0.8950190       -2.2168450       -1.7641530
H        -0.2798470       -2.5814930       -2.5991470
H        -1.9207460       -2.5501240       -1.9780250
C        -0.4705810       -2.8458310       -0.4712580
C        -0.2481630       -4.2200010       -0.3715460
C         0.0490220       -4.7704140        0.8722250
H        -0.3186150       -4.8429170       -1.2638350
C        -0.1030520       -2.5717460        1.8148510
C         0.1114580       -3.9307520        1.9878230
H         0.2254030       -5.8426820        0.9722000
H        -0.0507450       -1.8756350        2.6520540
H         0.3312030       -4.3175480        2.9830060
C         1.5694840        1.6925570       -0.3639890
H         2.3463030        1.9391480       -1.0995730
H         1.9550210        2.0066870        0.6158480
C         2.3007300       -0.4213850        0.6779580
H         2.0495340       -1.4846580        0.7167670
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H        2.0765090        0.0209930        1.6552280
C        0.3154810        2.4705580       -0.6064930
C        0.3400020        3.7900500       -1.0503630
C       -1.9952940        2.5638200       -0.2874280
C       -0.8532520        4.5084580       -1.0998080
H        1.2881770        4.2449820       -1.3381970
C       -2.0384150        3.8878400       -0.6963750
H       -2.8990830        2.0494910        0.0323890
H       -0.8580690        5.5444060       -1.4427590
H       -2.9916710        4.4161220       -0.7020860
C        3.7556220       -0.2427750        0.3246680
C        4.4165990       -1.1939970       -0.4698590
C        4.4778790        0.8647200        0.7983000
C        5.7615240       -1.0281340       -0.8051570
H        3.8819530       -2.0802350       -0.8189920
C        5.8230530        1.0315310        0.4639120
H        3.9935470        1.5969170        1.4482360
C        6.4655970        0.0885760       -0.3440810
H        6.2628440       -1.7773640       -1.4214070
H        6.3724750        1.8959090        0.8426680
H        7.5184160        0.2177670       -0.6045210
N       -2.6021700       -0.3594460        0.1562160
N       -0.3764030       -2.0422380        0.6032690
N       -0.8394620        1.8652880       -0.2561240
Mn      -0.6286290       -0.0472490        0.3055450
O       -0.4805830        0.1993630        1.8658540
C       -0.8900340        2.4626540        3.0437870
H       -0.6480200        1.3732840        2.4427810
H       -1.9828730        2.4843260        2.9291640
H       -0.5133830        2.1839670        4.0411910
O       -0.2944660        3.4929420        2.4319760
H        0.6126040        3.6261370        2.7585520
63
Singlet_TS_MnBnTPEN_Oxo_G2.log
63
Final Energy =            -2545.9037860800
C       -2.7964330       -1.0020440        0.4672670
C       -1.4822190       -1.1356410        2.4035270
C       -2.5313170       -1.7066260        3.1170190
C       -3.7484300       -1.9247030        2.4693450
C       -3.8811200       -1.5736250        1.1235520
H       -0.5104730       -0.9414310        2.8595580
H       -2.3867160       -1.9756160        4.1635490
H       -4.5872200       -2.3740710        3.0035780
H       -4.8115640       -1.7463120        0.5817320
C       -2.8111520       -0.5716790       -0.9770940
H       -3.0741970        0.4916640       -1.0622580
H       -3.5535900       -1.1359690       -1.5603000
N       -1.4370700       -0.7735870       -1.5107730
C       -1.1253860       -0.0040910       -2.7428670
H       -1.5215590       -0.5079690       -3.6370430
H       -1.6200440        0.9738720       -2.6817920
C        0.3818190        0.1310180       -2.8277240
H        0.8575260       -0.8569520       -2.8536150
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H        0.6862900         0.6614680        -3.7411200
N        0.8835330         0.8607270        -1.6132230
C       -1.1952740        -2.2336120        -1.7057370
H       -1.2311770        -2.4851850        -2.7753100
H       -2.0125320        -2.7954020        -1.2312530
C        0.0870680        -2.6829340        -1.0834770
C        0.6347530        -3.9386990        -1.3466350
C        1.7810970        -4.3337030        -0.6622200
H        0.1552350        -4.5922630        -2.0760820
C        1.7463970        -2.2253080         0.4793430
C        2.3397220        -3.4628020         0.2767860
H        2.2294980        -5.3102400        -0.8525260
H        2.1427510        -1.5185360         1.2057090
H        3.2278180        -3.7310090         0.8493540
C        0.5704420         2.3174570        -1.7535310
H        0.4083130         2.5650970        -2.8124600
H        1.4431990         2.9115360        -1.4500600
C        2.3476020         0.6588230        -1.4610390
H        2.8728170         1.2549070        -2.2304800
H        2.5771950        -0.3905990        -1.6875060
C       -0.6056630         2.7306360        -0.9256510
C       -1.1445500         4.0127650        -1.0140360
C       -2.0620250         2.1853980         0.8183590
C       -2.1743510         4.3758770        -0.1499170
H       -0.7473160         4.7144380        -1.7481610
C       -2.6297830         3.4487140         0.7926380
H       -2.3924870         1.4410200         1.5390310
H       -2.6109040         5.3746160        -0.2028070
H       -3.4191540         3.6961170         1.5022800
C        2.9244110         0.9873410        -0.1116260
C        2.1598220         1.6681750         0.9207150
C        4.1859640         0.5050750         0.2066300
C        2.7461580         1.8650000         2.2237210
H        1.4265910         2.4248220         0.6436460
C        4.7147320         0.6923240         1.4905320
H        4.7630030        -0.0471530        -0.5371650
C        3.9944030         1.3688860         2.5041740
H        2.1687790         2.4125360         2.9699970
H        5.7036800         0.2886370         1.7175460
H        4.4411610         1.5017510         3.4900560
N       -1.6245240        -0.7896480         1.1130840
N        0.6494840        -1.8363140        -0.2032950
N       -1.0798070         1.8242250        -0.0405770
Mn      -0.1759400         0.0463560         0.0016620
O        0.9340180         0.3284230         1.1454390
63
Singlet_TS_MnBnTPEN_Oxo_G3.log
63
Final Energy =            -2545.8778248300
C       -2.8197300         1.0964470         0.3281040
C       -2.0599080         0.1317130         2.3249650
C       -3.2543600         0.4422030         2.9678970
C       -4.2542980         1.1026470         2.2511330
C       -4.0380770         1.4295410         0.9097250
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H	-1.2439930	-0.3838840	2.8346060
H	-3.3920270	0.1639790	4.0129080
H	-5.2019490	1.3549450	2.7298990
H	-4.8028050	1.9329620	0.3175290
C	-2.4359430	1.4096540	-1.0940370
H	-1.8867650	2.3604250	-1.1422520
H	-3.3157910	1.5098770	-1.7453490
N	-1.5423780	0.3134920	-1.5831710
C	-0.7503610	0.6756280	-2.7891400
H	-1.3546490	0.5718490	-3.7016600
H	-0.4560110	1.7305440	-2.7144440
C	0.4517560	-0.2416850	-2.8166320
H	0.1382790	-1.2934800	-2.8598540
H	1.0839250	-0.0560450	-3.6973300
N	1.2407690	-0.0423410	-1.5594340
C	-2.3579420	-0.9223020	-1.8202740
H	-2.3668090	-1.1594940	-2.8930230
H	-3.4029030	-0.7182580	-1.5471770
C	-1.8760490	-2.0917230	-1.0215800
C	-2.4239110	-3.3637530	-1.1879500
C	-1.9800110	-4.4019270	-0.3736730
H	-3.1927130	-3.5249540	-1.9446010
C	-0.5002990	-2.8450710	0.6940450
C	-1.0046260	-4.1339050	0.5901890
H	-2.3928560	-5.4060030	-0.4848110
H	0.2555280	-2.5947750	1.4369150
H	-0.6327900	-4.9108810	1.2582880
C	2.0278020	1.2246500	-1.6468520
H	2.1650070	1.5200480	-2.6968640
H	3.0386570	1.0506730	-1.2504450
C	2.1550310	-1.1998460	-1.3561620
H	2.8111590	-1.3075050	-2.2331930
H	1.5376210	-2.1093180	-1.3023390
C	1.4132810	2.3315810	-0.8511700
C	1.8678060	3.6449780	-0.9480960
C	-0.0550000	2.9139670	0.8690400
C	1.3343850	4.6107900	-0.0973990
H	2.6388230	3.8956960	-1.6772670
C	0.3660680	4.2336010	0.8381070
H	-0.8132560	2.5864160	1.5771650
H	1.6757900	5.6456330	-0.1567270
H	-0.0665220	4.9520800	1.5341790
C	2.9969770	-1.0998600	-0.1133420
C	2.4148290	-0.8031680	1.1536460
C	4.3565780	-1.3808870	-0.1286540
C	3.1428810	-0.9104240	2.3653650
H	1.9721160	0.3406070	1.3320930
C	5.1061860	-1.4116150	1.0601240
H	4.8449980	-1.5954410	-1.0807520
C	4.5056580	-1.1792010	2.3001400
H	2.6265130	-0.7337920	3.3098660
H	6.1734140	-1.6337280	1.0088610
H	5.0924850	-1.2235110	3.2183430
N	-1.8587080	0.4628690	1.0399770

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N       -0.9212080      -1.8441970      -0.1073240
N        0.4461980       1.9794460       0.0255290
Mn      -0.2003410       0.0750710      -0.0247470
O        0.9938740      -0.5623150       1.2527450
63
Singlet_TS_MnBnTPEN_Oxo_G4.log
63
Final Energy =          -2545.9037860400
C       -2.7969030      -1.0008770       0.4672040
C       -1.4828280      -1.1347350       2.4035350
C       -2.5321890      -1.7051870       3.1170650
C       -3.7493630      -1.9228620       2.4693710
C       -3.8818520      -1.5719240       1.1235230
H       -0.5110140      -0.9408660       2.8595640
H       -2.3877400      -1.9740860       4.1636390
H       -4.5883570      -2.3718100       3.0036350
H       -4.8123420      -1.7443040       0.5816880
C       -2.8114110      -0.5707080      -0.9772170
H       -3.0740780       0.4927160      -1.0625460
H       -3.5540440      -1.1348230      -1.5603520
N       -1.4373940      -0.7731740      -1.5108400
C       -1.1253690      -0.0038620      -2.7429630
H       -1.5218350      -0.5075420      -3.6371210
H       -1.6195010       0.9743700      -2.6818950
C        0.3819010       0.1304590      -2.8278200
H        0.8570920      -0.8577630      -2.8535500
H        0.6866730       0.6606420      -3.7412710
N        0.8839120       0.8600570      -1.6133840
C       -1.1961330      -2.2332990      -1.7057380
H       -1.2319170      -2.4848550      -2.7753210
H       -2.0136990      -2.7947710      -1.2314130
C        0.0859270      -2.6831250      -1.0832520
C        0.6330600      -3.9391770      -1.3461970
C        1.7791550      -4.3346240      -0.6616230
H        0.1533230      -4.5926160      -2.0756120
C        1.7453050      -2.2260770       0.4796790
C        2.3380910      -3.4638620       0.2773270
H        2.2271230      -5.3113920      -0.8517610
H        2.1418810      -1.5194060       1.2060200
H        3.2260050      -3.7324040       0.8500200
C        0.5715440       2.3169290      -1.7538710
H        0.4091790       2.5644350      -2.8127940
H        1.4447350       2.9105720      -1.4508060
C        2.3478670       0.6574820      -1.4610800
H        2.8734210       1.2532110      -2.2305620
H        2.5769890      -0.3920790      -1.6873660
C       -0.6041260       2.7309040      -0.9257690
C       -1.1419750       4.0134830      -1.0139320
C       -2.0610120       2.1864590       0.8180420
C       -2.1715810       4.3772130      -0.1498390
H       -0.7440750       4.7149870      -1.7478650
C       -2.6278320       3.4501990       0.7924730
H       -2.3920210       1.4422280       1.5386170
H       -2.6073510       5.3763030      -0.2025520
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H	-3.4170890	3.6980700	1.5020790
C	2.9246920	0.9859650	-0.1116680
C	2.1602700	1.6673200	0.9204740
C	4.1859920	0.5032110	0.2068210
C	2.7465800	1.8641840	2.2235010
H	1.4274210	2.4241980	0.6431980
C	4.7147080	0.6904930	1.4907440
H	4.7628760	-0.0494200	-0.5367960
C	3.9945800	1.3675910	2.5041750
H	2.1693710	2.4121390	2.9696000
H	5.7034520	0.2864090	1.7179430
H	4.4413070	1.5004760	3.4900690
N	-1.6249340	-0.7888700	1.1130360
N	0.6486330	-1.8366610	-0.2031100
N	-1.0789960	1.8246970	-0.0408800
Mn	-0.1759910	0.0464090	0.0015620
O	0.9341060	0.3281730	1.1453650

63

TS$_{SRN1}$

63

Final Energy =   -2545.9391103200

C	-2.6552380	-1.3917240	0.4522270
C	-1.3311660	-1.2710890	2.3987830
C	-2.2927200	-1.9541250	3.1332940
C	-3.4680660	-2.3572360	2.4954400
C	-3.6505030	-2.0767630	1.1380190
H	-0.3959270	-0.9178250	2.8353100
H	-2.1165590	-2.1619040	4.1886820
H	-4.2392580	-2.8957170	3.0489270
H	-4.5517710	-2.3911980	0.6111320
C	-2.7295140	-1.0113870	-1.0048690
H	-3.1667560	-0.0088100	-1.1158920
H	-3.3647840	-1.7067450	-1.5722660
N	-1.3395500	-0.9940370	-1.5240290
C	-1.1270760	-0.1858440	-2.7540590
H	-1.4333670	-0.7437580	-3.6511360
H	-1.7625530	0.7074110	-2.6977280
C	0.3443160	0.1753050	-2.8326140
H	0.9695530	-0.7245770	-2.8777850
H	0.5640240	0.7623030	-3.7356460
N	0.7464460	0.9611880	-1.6098480
C	-0.8447760	-2.3938350	-1.6910940
H	-0.8698230	-2.6852300	-2.7507590
H	-1.5341280	-3.0754240	-1.1707380
C	0.5137770	-2.5960860	-1.0937270
C	1.2878860	-3.7237130	-1.3561000
C	2.4812110	-3.9025800	-0.6574330
H	0.9463590	-4.4536950	-2.0906330
C	2.0565750	-1.8497330	0.5055070
C	2.8630000	-2.9584190	0.3004870
H	3.1024630	-4.7789360	-0.8502510
H	2.2898000	-1.0818850	1.2398140
H	3.7770260	-3.0721770	0.8833250
C	0.2256580	2.3655100	-1.7348600

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H           0.0439410          2.5946530         -2.7951790
H           1.0057120          3.0695390         -1.4172240
C           2.2347370          0.9747330         -1.4763150
H           2.6375710          1.6790000         -2.2254040
H           2.6083590         -0.0157470         -1.7635450
C          -1.0048420          2.6093540         -0.9183420
C          -1.7070540          3.8105920         -1.0068250
C          -2.3922910          1.8695980          0.8086960
C          -2.7857290          4.0297290         -0.1546440
H          -1.3953240          4.5633080         -1.7315100
C          -3.1255500          3.0451800          0.7773070
H          -2.6252430          1.0873240          1.5262630
H          -3.3489190          4.9628330         -0.2079910
H          -3.9495920          3.1794670          1.4779200
C           2.7734480          1.3137770         -0.1090940
C           1.9756440          1.9559280          0.9140590
C           4.0603460          0.9017780          0.2071870
C           2.5578810          2.2005320          2.2067630
H           1.1757560          2.6389140          0.6349460
C           4.5936230          1.1304130          1.4845790
H           4.6603750          0.3764760         -0.5382100
C           3.8354300          1.7790830          2.4875370
H           1.9548870          2.7211580          2.9518160
H           5.6056280          0.7883210          1.7091070
H           4.2739700          1.9545450          3.4708960
N          -1.5239270         -1.0007920          1.0948080
N           0.9219390         -1.6668820         -0.2027350
N          -1.3657780          1.6488420         -0.0415280
Mn         -0.2019790         -0.0144860         -0.0226740
O           0.7475130          0.5523040          1.2555590
63
OSS_TS_MnBnTPEN_Oxo_G1.log
63
Final Energy =        -2545.9053440100
C          -2.2682760          1.9154570          0.2355650
C          -1.7804520          0.9294400          2.3103840
C          -2.7530890          1.6953540          2.9428990
C          -3.4975870          2.5997070          2.1834730
C          -3.2559390          2.7067250          0.8113970
H          -1.1619980          0.2127970          2.8522050
H          -2.9178370          1.5784010          4.0141210
H          -4.2688930          3.2127420          2.6527120
H          -3.8308020          3.3912350          0.1871870
C          -1.9111750          1.9455480         -1.2304260
H          -1.0877200          2.6498430         -1.4107250
H          -2.7608850          2.2743280         -1.8466360
N          -1.4666290          0.5783360         -1.5949300
C          -0.6494900          0.4665900         -2.8322980
H          -1.2879290          0.4466760         -3.7272480
H          -0.0119040          1.3558980         -2.9154720
C           0.1749170         -0.8053170         -2.7291700
H          -0.4624280         -1.6898150         -2.6046250
H           0.7769010         -0.9663620         -3.6354400
N           1.0707810         -0.6916410         -1.5297550
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C     -2.6494020     -0.3264830     -1.6743570
H     -2.9123490     -0.5233700     -2.7230500
H     -3.5180330      0.1848340     -1.2333200
C     -2.4545540     -1.5880060     -0.9002670
C     -3.3274720     -2.6688800     -1.0191690
C     -3.2183250     -3.7296380     -0.1238760
H     -4.0957170     -2.6558700     -1.7932600
C     -1.4117810     -2.5637000      0.9350690
C     -2.2614100     -3.6585200      0.8921900
H     -3.8893940     -4.5869640     -0.1984700
H     -0.6853140     -2.4481940      1.7348750
H     -2.1689130     -4.4377270      1.6487650
C      2.1395280      0.3169390     -1.8385620
H      2.1756340      0.5043520     -2.9205290
H      3.1206020     -0.0924050     -1.5796890
C      1.6942040     -2.0344020     -1.1979000
H      2.2809070     -2.3628590     -2.0684870
H      0.8696400     -2.7425380     -1.0492990
C      1.9782150      1.5948730     -1.0847030
C      2.8649650      2.6564520     -1.2660430
C      0.8633670      2.7493840      0.6094230
C      2.7294080      3.7932620     -0.4762480
H      3.6559370      2.5739690     -2.0122770
C      1.7174070      3.8325150      0.4887570
H      0.0740110      2.7467360      1.3561340
H      3.4121580      4.6354720     -0.6005000
H      1.5869180      4.6919490      1.1462600
C      2.5591160     -1.9322760      0.0215710
C      3.9206390     -1.6758600     -0.0450850
C      1.9320870     -2.0018330      1.3129830
C      4.6497550     -1.4133480      1.1288300
H      4.4391390     -1.6728050     -1.0055880
C      2.6923960     -1.7245940      2.4955430
H      1.1067770     -2.7066490      1.4119620
C      4.0315980     -1.4130020      2.3959090
H      5.7161940     -1.1921150      1.0513100
H      2.1938570     -1.7826180      3.4644740
H      4.6205210     -1.1972730      3.2882390
N     -1.5480520      1.0491070      0.9915090
N     -1.4721400     -1.5711840      0.0222380
N      0.9779350      1.6588100     -0.1843820
Mn    -0.1536770      0.0004990     -0.0039120
O      0.6109610     -0.5720580      1.3257600
63
OSS_TS_MnBnTPEN_Oxo_G2.log
63
Final Energy =          -2545.9134789800
C     -2.7017230     -1.2408070      0.4814260
C     -1.3623050     -1.2287850      2.4118920
C     -2.3577420     -1.8626670      3.1467200
C     -3.5605800     -2.1855270      2.5156940
C     -3.7322420     -1.8766360      1.1637650
H     -0.4049560     -0.9482160      2.8528870
H     -2.1844070     -2.0964730      4.1972310
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H	-4.3585960	-2.6844590	3.0681200
H	-4.6519840	-2.1313320	0.6365310
C	-2.7646760	-0.8480740	-0.9732430
H	-3.1327330	0.1819410	-1.0789630
H	-3.4510240	-1.4958520	-1.5376270
N	-1.3802260	-0.9264840	-1.5036450
C	-1.1279200	-0.1483420	-2.7448930
H	-1.4718550	-0.6969190	-3.6341040
H	-1.7078910	0.7822510	-2.6978150
C	0.3623300	0.1238750	-2.8305370
H	0.9317640	-0.8130360	-2.8541180
H	0.6159780	0.6794690	-3.7444940
N	0.7961550	0.9084550	-1.6202750
C	-0.9918090	-2.3583780	-1.6700280
H	-1.0352600	-2.6452550	-2.7303490
H	-1.7299510	-2.9885800	-1.1526670
C	0.3480080	-2.6545050	-1.0748800
C	1.0284530	-3.8439200	-1.3299260
C	2.2161460	-4.1032900	-0.6497640
H	0.6182550	-4.5545490	-2.0479300
C	1.9633920	-2.0022630	0.4777210
C	2.6829810	-3.1711550	0.2812600
H	2.7665910	-5.0270040	-0.8361240
H	2.2797730	-1.2477200	1.1947230
H	3.5967700	-3.3401050	0.8511310
C	0.3420100	2.3297470	-1.7776950
H	0.1445110	2.5379820	-2.8392720
H	1.1596100	3.0081200	-1.5004460
C	2.2773140	0.8496460	-1.4649640
H	2.7316380	1.5105030	-2.2257040
H	2.6070630	-0.1660270	-1.7152310
C	-0.8592750	2.6486140	-0.9442130
C	-1.4968920	3.8847580	-1.0338960
C	-2.2713090	1.9915170	0.7966870
C	-2.5554080	4.1652550	-0.1742890
H	-1.1529520	4.6158900	-1.7661840
C	-2.9401890	3.2043800	0.7654640
H	-2.5414830	1.2256550	1.5193680
H	-3.0683540	5.1269060	-0.2283360
H	-3.7501150	3.3867580	1.4716280
C	2.8204980	1.2128070	-0.1090830
C	2.0684210	1.9566850	0.8705710
C	4.0765260	0.7275260	0.2470630
C	2.6272040	2.2034100	2.1631980
H	1.2496470	2.6083900	0.5767890
C	4.5942890	0.9693310	1.5226980
H	4.6511660	0.1310560	-0.4636630
C	3.8664170	1.7023550	2.4888530
H	2.0486320	2.7928820	2.8755270
H	5.5751880	0.5661560	1.7824910
H	4.2968410	1.8757840	3.4758940
N	-1.5439530	-0.9236170	1.1142590
N	0.8303190	-1.7420950	-0.2084490
N	-1.2617900	1.7109220	-0.0589000

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Mn        -0.1839460        0.0131780       -0.0136050
O          0.8214670        0.4515900        1.1870370
63
Quintet_TS_HAT_MnBnTPEN_Oxo_G1.log
63
Final Energy =            -2545.9061093900
C         -3.2059100        0.1889370        0.1954660
C         -2.2879510       -0.3555660        2.2999580
C         -3.5539900       -0.4174300        2.8688900
C         -4.6686160       -0.1645570        2.0662640
C         -4.4934560        0.1389330        0.7124530
H         -1.3732570       -0.5321200        2.8676530
H         -3.6555090       -0.6611670        3.9264010
H         -5.6737770       -0.2101070        2.4887230
H         -5.3449230        0.3297770        0.0589550
C         -2.8649580        0.5292560       -1.2295010
H         -2.6969120        1.6103490       -1.3324040
H         -3.6763130        0.2616260       -1.9214490
N         -1.6079950       -0.1879400       -1.5679070
C         -0.8497230        0.4043250       -2.7004080
H         -1.3009030        0.1221030       -3.6636000
H         -0.9070830        1.4969300       -2.6271420
C          0.5738810       -0.0986980       -2.6210440
H          0.6067030       -1.1904750       -2.7292680
H          1.1841850        0.3214920       -3.4325260
N          1.2149780        0.2422580       -1.2954000
C         -1.8964650       -1.6406110       -1.7894980
H         -1.8577080       -1.8749490       -2.8630050
H         -2.9284940       -1.8462550       -1.4695000
C         -0.9933850       -2.5393490       -1.0024690
C         -0.9357440       -3.9132790       -1.2245950
C         -0.1618000       -4.7043620       -0.3776300
H         -1.5030470       -4.3500190       -2.0468880
C          0.4445880       -2.7310150        0.8423030
C          0.5289340       -4.1045210        0.6801660
H         -0.1044550       -5.7826470       -0.5355110
H          0.9582960       -2.2077900        1.6472700
H          1.1319100       -4.6898900        1.3741550
C          1.6404220        1.6753860       -1.2800020
H          1.9993750        1.9723310       -2.2758520
H          2.4959370        1.7731990       -0.5958370
C          2.4116090       -0.6611270       -1.1583010
H          2.9469560       -0.6413690       -2.1189050
H          2.0355620       -1.6854710       -1.0329340
C          0.5728980        2.5924990       -0.7789780
C          0.6328280        3.9689710       -0.9887290
C         -1.2807230        2.8384930        0.6246550
C         -0.2986380        4.7921890       -0.3603830
H          1.4143510        4.3807440       -1.6277860
C         -1.2605190        4.2170290        0.4740630
H         -2.0197070        2.3592960        1.2630420
H         -0.2679480        5.8725190       -0.5105740
H         -1.9968190        4.8226080        1.0022670
C          3.3870000       -0.3292930       -0.0618420
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C          3.0195840          0.1014810          1.2186690
C          4.7570330         -0.5549760         -0.2558140
C          3.9036820          0.5325320          2.2020520
H          1.7991790         -0.0334000          1.5342300
C          5.6774430         -0.2520130          0.7562570
H          5.1065790         -0.9532770         -1.2111140
C          5.2612600          0.2834910          1.9839630
H          3.5487310          0.9834440          3.1307210
H          6.7428540         -0.3945300          0.5646010
H          5.9901440          0.5257400          2.7598610
N         -2.1365230         -0.0557130          0.9969950
N         -0.2883920         -1.9700690         -0.0012320
N         -0.3951960          2.0439770         -0.0127200
Mn        -0.3529430          0.0216450          0.1231280
O          0.5382340          0.0490320          1.6105340
63
Singlet_TS_HAT_MnBnTPEN_Oxo_G1.log
63
Final Energy =               -2545.9085541600
C          3.0669470          0.1881540         -0.3123920
C          2.0701710         -0.6342440         -2.2762820
C          3.3133680         -0.8084350         -2.8707620
C          4.4624750         -0.4697050         -2.1547210
C          4.3361980          0.0297190         -0.8573640
H          1.1500510         -0.8832100         -2.8035450
H          3.3662930         -1.2076100         -3.8837610
H          5.4506280         -0.6010170         -2.5984380
H          5.2104730          0.2934880         -0.2617560
C          2.8031460          0.7492650          1.0530200
H          2.6708900          1.8386730          0.9957710
H          3.6451380          0.5683720          1.7354600
N          1.5525800          0.1342580          1.5596050
C          0.8730310          0.9375500          2.6076360
H          1.3734280          0.8197990          3.5811570
H          0.9338270          1.9992450          2.3451550
C         -0.5486270          0.4393430          2.6817430
H         -0.5757880         -0.6090850          3.0047360
H         -1.1394790          1.0161510          3.4064490
N         -1.2131430          0.5083820          1.3333800
C          1.8287850         -1.2454720          2.0593740
H          1.6111330         -1.3098860          3.1344850
H          2.9030960         -1.4576270          1.9620850
C          1.0803530         -2.2934290          1.3033270
C          1.2074300         -3.6462910          1.6239690
C          0.6061280         -4.5992750          0.8095760
H          1.7964000         -3.9336430          2.4955960
C         -0.1961130         -2.8169670         -0.5779170
C         -0.0892240         -4.1741830         -0.3263460
H          0.6962830         -5.6613220          1.0429380
H         -0.7206650         -2.4502480         -1.4572440
H         -0.5501820         -4.8811740         -1.0162940
C         -1.6591900          1.8999700          1.0402620
H         -2.1045570          2.3576470          1.9339560
H         -2.4414770          1.8475190          0.2710980
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C      -2.4195210      -0.4360390       1.3923440
H      -2.9662510      -0.1336820       2.2992610
H      -2.0115800      -1.4365270       1.5697450
C      -0.5708790       2.7347950       0.4613230
C      -0.5744590       4.1246800       0.5179850
C       1.2680740       2.7441190      -0.9897100
C       0.3818990       4.8321880      -0.2083870
H      -1.3294490       4.6350600       1.1158720
C       1.3033350       4.1289730      -0.9903970
H       1.9712460       2.1695700      -1.5861520
H       0.4017920       5.9226990      -0.1750820
H       2.0502950       4.6417260      -1.5960460
C      -3.3489240      -0.4327360       0.2157540
C      -3.3056360      -1.4874330      -0.7175100
C      -4.3342240       0.5623440       0.0570160
C      -4.1592300      -1.5080080      -1.8210330
H      -2.6272810      -2.3214360      -0.5497590
C      -5.1869610       0.5436890      -1.0443590
H      -4.4532710       1.3448700       0.8087160
C      -5.0902890      -0.4828890      -1.9957400
H      -4.1052590      -2.3334810      -2.5330260
H      -5.9416730       1.3241480      -1.1574880
H      -5.7618900      -0.4927950      -2.8566280
N       1.9623210      -0.1373540      -1.0266730
N       0.3464090      -1.8927580       0.2507570
N       0.3628070       2.0624400      -0.2517100
Mn      0.1703970       0.0880050      -0.1648350
O      -0.8184100      -0.1586530      -1.2807940
63
Singlet_TS_MnBnTPEN_Oxo_G2.log
63
Final Energy =           -2545.9037860800
C      -2.7964330      -1.0020440       0.4672670
C      -1.4822190      -1.1356410       2.4035270
C      -2.5313170      -1.7066260       3.1170190
C      -3.7484300      -1.9247030       2.4693450
C      -3.8811200      -1.5736250       1.1235520
H      -0.5104730      -0.9414310       2.8595580
H      -2.3867160      -1.9756160       4.1635490
H      -4.5872200      -2.3740710       3.0035780
H      -4.8115640      -1.7463120       0.5817320
C      -2.8111520      -0.5716790      -0.9770940
H      -3.0741970       0.4916640      -1.0622580
H      -3.5535900      -1.1359690      -1.5603000
N      -1.4370700      -0.7735870      -1.5107730
C      -1.1253860      -0.0040910      -2.7428670
H      -1.5215590      -0.5079690      -3.6370430
H      -1.6200440       0.9738720      -2.6817920
C       0.3818190       0.1310180      -2.8277240
H       0.8575260      -0.8569520      -2.8536150
H       0.6862900       0.6614680      -3.7411200
N       0.8835330       0.8607270      -1.6132230
C      -1.1952740      -2.2336120      -1.7057370
H      -1.2311770      -2.4851850      -2.7753100
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H       -2.0125320      -2.7954020      -1.2312530
C        0.0870680      -2.6829340      -1.0834770
C        0.6347530      -3.9386990      -1.3466350
C        1.7810970      -4.3337030      -0.6622200
H        0.1552350      -4.5922630      -2.0760820
C        1.7463970      -2.2253080       0.4793430
C        2.3397220      -3.4628020       0.2767860
H        2.2294980      -5.3102400      -0.8525260
H        2.1427510      -1.5185360       1.2057090
H        3.2278180      -3.7310090       0.8493540
C        0.5704420       2.3174570      -1.7535310
H        0.4083130       2.5650970      -2.8124600
H        1.4431990       2.9115360      -1.4500600
C        2.3476020       0.6588230      -1.4610390
H        2.8728170       1.2549070      -2.2304800
H        2.5771950      -0.3905990      -1.6875060
C       -0.6056630       2.7306360      -0.9256510
C       -1.1445500       4.0127650      -1.0140360
C       -2.0620250       2.1853980       0.8183590
C       -2.1743510       4.3758770      -0.1499170
H       -0.7473160       4.7144380      -1.7481610
C       -2.6297830       3.4487140       0.7926380
H       -2.3924870       1.4410200       1.5390310
H       -2.6109040       5.3746160      -0.2028070
H       -3.4191540       3.6961170       1.5022800
C        2.9244110       0.9873410      -0.1116260
C        2.1598220       1.6681750       0.9207150
C        4.1859640       0.5050750       0.2066300
C        2.7461580       1.8650000       2.2237210
H        1.4265910       2.4248220       0.6436460
C        4.7147320       0.6923240       1.4905320
H        4.7630030      -0.0471530      -0.5371650
C        3.9944030       1.3688860       2.5041740
H        2.1687790       2.4125360       2.9699970
H        5.7036800       0.2886370       1.7175460
H        4.4411610       1.5017510       3.4900560
N       -1.6245240      -0.7896480       1.1130840
N        0.6494840      -1.8363140      -0.2032950
N       -1.0798070       1.8242250      -0.0405770
Mn      -0.1759400       0.0463560       0.0016620
O        0.9340180       0.3284230       1.1454390
63
Singlet_TS_MnBnTPEN_Oxo_G3.log
63
Final Energy =          -2545.8778248300
C       -2.8197300       1.0964470       0.3281040
C       -2.0599080       0.1317130       2.3249650
C       -3.2543600       0.4422030       2.9678970
C       -4.2542980       1.1026470       2.2511330
C       -4.0380770       1.4295410       0.9097250
H       -1.2439930      -0.3838840       2.8346060
H       -3.3920270       0.1639790       4.0129080
H       -5.2019490       1.3549450       2.7298990
H       -4.8028050       1.9329620       0.3175290
```

```
C     -2.4359430      1.4096540     -1.0940370
H     -1.8867650      2.3604250     -1.1422520
H     -3.3157910      1.5098770     -1.7453490
N     -1.5423780      0.3134920     -1.5831710
C     -0.7503610      0.6756280     -2.7891400
H     -1.3546490      0.5718490     -3.7016600
H     -0.4560110      1.7305440     -2.7144440
C      0.4517560     -0.2416850     -2.8166320
H      0.1382790     -1.2934800     -2.8598540
H      1.0839250     -0.0560450     -3.6973300
N      1.2407690     -0.0423410     -1.5594340
C     -2.3579420     -0.9223020     -1.8202740
H     -2.3668090     -1.1594940     -2.8930230
H     -3.4029030     -0.7182580     -1.5471770
C     -1.8760490     -2.0917230     -1.0215800
C     -2.4239110     -3.3637530     -1.1879500
C     -1.9800110     -4.4019270     -0.3736730
H     -3.1927130     -3.5249540     -1.9446010
C     -0.5002990     -2.8450710      0.6940450
C     -1.0046260     -4.1339050      0.5901890
H     -2.3928560     -5.4060030     -0.4848110
H      0.2555280     -2.5947750      1.4369150
H     -0.6327900     -4.9108810      1.2582880
C      2.0278020      1.2246500     -1.6468520
H      2.1650070      1.5200480     -2.6968640
H      3.0386570      1.0506730     -1.2504450
C      2.1550310     -1.1998460     -1.3561620
H      2.8111590     -1.3075050     -2.2331930
H      1.5376210     -2.1093180     -1.3023390
C      1.4132810      2.3315810     -0.8511700
C      1.8678060      3.6449780     -0.9480960
C     -0.0550000      2.9139670      0.8690400
C      1.3343850      4.6107900     -0.0973990
H      2.6388230      3.8956960     -1.6772670
C      0.3660680      4.2336010      0.8381070
H     -0.8132560      2.5864160      1.5771650
H      1.6757900      5.6456330     -0.1567270
H     -0.0665220      4.9520800      1.5341790
C      2.9969770     -1.0998600     -0.1133420
C      2.4148290     -0.8031680      1.1536460
C      4.3565780     -1.3808870     -0.1286540
C      3.1428810     -0.9104240      2.3653650
H      1.9721160      0.3406070      1.3320930
C      5.1061860     -1.4116150      1.0601240
H      4.8449980     -1.5954410     -1.0807520
C      4.5056580     -1.1792010      2.3001400
H      2.6265130     -0.7337920      3.3098660
H      6.1734140     -1.6337280      1.0088610
H      5.0924850     -1.2235110      3.2183430
N     -1.8587080      0.4628690      1.0399770
N     -0.9212080     -1.8441970     -0.1073240
N      0.4461980      1.9794460      0.0255290
Mn    -0.2003410      0.0750710     -0.0247470
O      0.9938740     -0.5623150      1.2527450
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63
Singlet_TS_MnBnTPEN_Oxo_G4.log
63
Final Energy =        -2545.9037860400
C       -2.7969030      -1.0008770       0.4672040
C       -1.4828280      -1.1347350       2.4035350
C       -2.5321890      -1.7051870       3.1170650
C       -3.7493630      -1.9228620       2.4693710
C       -3.8818520      -1.5719240       1.1235230
H       -0.5110140      -0.9408660       2.8595640
H       -2.3877400      -1.9740860       4.1636390
H       -4.5883570      -2.3718100       3.0036350
H       -4.8123420      -1.7443040       0.5816880
C       -2.8114110      -0.5707080      -0.9772170
H       -3.0740780       0.4927160      -1.0625460
H       -3.5540440      -1.1348230      -1.5603520
N       -1.4373940      -0.7731740      -1.5108400
C       -1.1253690      -0.0038620      -2.7429630
H       -1.5218350      -0.5075420      -3.6371210
H       -1.6195010       0.9743700      -2.6818950
C        0.3819010       0.1304590      -2.8278200
H        0.8570920      -0.8577630      -2.8535500
H        0.6866730       0.6606420      -3.7412710
N        0.8839120       0.8600570      -1.6133840
C       -1.1961330      -2.2332990      -1.7057380
H       -1.2319170      -2.4848550      -2.7753210
H       -2.0136990      -2.7947710      -1.2314130
C        0.0859270      -2.6831250      -1.0832520
C        0.6330600      -3.9391770      -1.3461970
C        1.7791550      -4.3346240      -0.6616230
H        0.1533230      -4.5926160      -2.0756120
C        1.7453050      -2.2260770       0.4796790
C        2.3380910      -3.4638620       0.2773270
H        2.2271230      -5.3113920      -0.8517610
H        2.1418810      -1.5194060       1.2060200
H        3.2260050      -3.7324040       0.8500200
C        0.5715440       2.3169290      -1.7538710
H        0.4091790       2.5644350      -2.8127940
H        1.4447350       2.9105720      -1.4508060
C        2.3478670       0.6574820      -1.4610800
H        2.8734210       1.2532110      -2.2305620
H        2.5769890      -0.3920790      -1.6873660
C       -0.6041260       2.7309040      -0.9257690
C       -1.1419750       4.0134830      -1.0139320
C       -2.0610120       2.1864590       0.8180420
C       -2.1715810       4.3772130      -0.1498390
H       -0.7440750       4.7149870      -1.7478650
C       -2.6278320       3.4501990       0.7924730
H       -2.3920210       1.4422280       1.5386170
H       -2.6073510       5.3763030      -0.2025520
H       -3.4170890       3.6980700       1.5020790
C        2.9246920       0.9859650      -0.1116680
C        2.1602700       1.6673200       0.9204740
C        4.1859920       0.5032110       0.2068210
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C	2.7465800	1.8641840	2.2235010
H	1.4274210	2.4241980	0.6431980
C	4.7147080	0.6904930	1.4907440
H	4.7628760	-0.0494200	-0.5367960
C	3.9945800	1.3675910	2.5041750
H	2.1693710	2.4121390	2.9696000
H	5.7034520	0.2864090	1.7179430
H	4.4413070	1.5004760	3.4900690
N	-1.6249340	-0.7888700	1.1130360
N	0.6486330	-1.8366610	-0.2031100
N	-1.0789960	1.8246970	-0.0408800
Mn	-0.1759910	0.0464090	0.0015620
O	0.9341060	0.3281730	1.1453650

63

TS$_{\text{HAT}}$

63

Final Energy =   -2545.9136245100

C	-3.2086010	0.0454930	0.2235780
C	-2.2476720	-0.4560550	2.3180400
C	-3.5037270	-0.5628630	2.9014360
C	-4.6365380	-0.3576550	2.1107560
C	-4.4875660	-0.0543540	0.7541440
H	-1.3247500	-0.5970640	2.8822590
H	-3.5830820	-0.8044930	3.9613270
H	-5.6343010	-0.4392060	2.5450960
H	-5.3520860	0.1006480	0.1082520
C	-2.9019910	0.4042600	-1.2034250
H	-2.7920050	1.4927610	-1.3069420
H	-3.7046730	0.0932810	-1.8872100
N	-1.6133770	-0.2476100	-1.5538960
C	-0.8967210	0.3833570	-2.6960170
H	-1.3454590	0.0746810	-3.6519060
H	-1.0088610	1.4715240	-2.6237350
C	0.5510580	-0.0457640	-2.6339720
H	0.6400280	-1.1330870	-2.7509370
H	1.1322030	0.4131030	-3.4458000
N	1.1835410	0.3181440	-1.3113120
C	-1.8333170	-1.7131960	-1.7779600
H	-1.8326560	-1.9334660	-2.8546170
H	-2.8356920	-1.9767150	-1.4097290
C	-0.8475130	-2.5641460	-1.0404730
C	-0.6893240	-3.9230570	-1.2995320
C	0.1531500	-4.6741920	-0.4812710
H	-1.2326410	-4.3817830	-2.1260440
C	0.6265670	-2.6929160	0.7838410
C	0.8086370	-4.0521090	0.5861130
H	0.2900750	-5.7404980	-0.6685360
H	1.1145330	-2.1551950	1.5951540
H	1.4618110	-4.6077590	1.2587540
C	1.5483650	1.7686470	-1.2821320
H	1.8923120	2.0882990	-2.2760700
H	2.3992460	1.8918510	-0.5965890
C	2.4240400	-0.5296280	-1.1721710
H	2.9749620	-0.4465720	-2.1204420

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H        2.0942410       -1.5729250       -1.0949000
C        0.4407050        2.6319520       -0.7732180
C        0.4298400        4.0105460       -0.9736280
C       -1.4187350        2.7751080        0.6413410
C       -0.5406460        4.7808250       -0.3370680
H        1.1870200        4.4658060       -1.6123000
C       -1.4683230        4.1531590        0.4985910
H       -2.1273140        2.2563680        1.2828650
H       -0.5663300        5.8620900       -0.4814090
H       -2.2310280        4.7178080        1.0345560
C        3.3622930       -0.1799710       -0.0458260
C        2.9829350        0.0636400        1.2674410
C        4.7485500       -0.1345930       -0.2892330
C        3.8277450        0.3136160        2.3300020
H        1.7492410        0.1344560        1.5198310
C        5.6524510        0.1121200        0.7459830
H        5.1094440       -0.2983430       -1.3079220
C        5.2037990        0.3362230        2.0496870
H        3.4499500        0.4903170        3.3384110
H        6.7220690        0.1333250        0.5287790
H        5.9114260        0.5338240        2.8577720
N       -2.1197290       -0.1548870        1.0118120
N       -0.1710850       -1.9690590       -0.0332790
N       -0.4977080        2.0308230       -0.0081480
Mn      -0.3474730        0.0136360        0.1080160
O        0.5226130        0.0816880        1.5794030
63
Triplet_TS_MnBnTPEN_Oxo_G2.log
63
Final Energy =          -2545.9391103200
C       -2.6552380       -1.3917240        0.4522270
C       -1.3311660       -1.2710890        2.3987830
C       -2.2927200       -1.9541250        3.1332940
C       -3.4680660       -2.3572360        2.4954400
C       -3.6505030       -2.0767630        1.1380190
H       -0.3959270       -0.9178250        2.8353100
H       -2.1165590       -2.1619040        4.1886820
H       -4.2392580       -2.8957170        3.0489270
H       -4.5517710       -2.3911980        0.6111320
C       -2.7295140       -1.0113870       -1.0048690
H       -3.1667560       -0.0088100       -1.1158920
H       -3.3647840       -1.7067450       -1.5722660
N       -1.3395500       -0.9940370       -1.5240290
C       -1.1270760       -0.1858440       -2.7540590
H       -1.4333670       -0.7437580       -3.6511360
H       -1.7625530        0.7074110       -2.6977280
C        0.3443160        0.1753050       -2.8326140
H        0.9695530       -0.7245770       -2.8777850
H        0.5640240        0.7623030       -3.7356460
N        0.7464460        0.9611880       -1.6098480
C       -0.8447760       -2.3938350       -1.6910940
H       -0.8698230       -2.6852300       -2.7507590
H       -1.5341280       -3.0754240       -1.1707380
C        0.5137770       -2.5960860       -1.0937270
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C      1.2878860     -3.7237130     -1.3561000
C      2.4812110     -3.9025800     -0.6574330
H      0.9463590     -4.4536950     -2.0906330
C      2.0565750     -1.8497330      0.5055070
C      2.8630000     -2.9584190      0.3004870
H      3.1024630     -4.7789360     -0.8502510
H      2.2898000     -1.0818850      1.2398140
H      3.7770260     -3.0721770      0.8833250
C      0.2256580      2.3655100     -1.7348600
H      0.0439410      2.5946530     -2.7951790
H      1.0057120      3.0695390     -1.4172240
C      2.2347370      0.9747330     -1.4763150
H      2.6375710      1.6790000     -2.2254040
H      2.6083590     -0.0157470     -1.7635450
C     -1.0048420      2.6093540     -0.9183420
C     -1.7070540      3.8105920     -1.0068250
C     -2.3922910      1.8695980      0.8086960
C     -2.7857290      4.0297290     -0.1546440
H     -1.3953240      4.5633080     -1.7315100
C     -3.1255500      3.0451800      0.7773070
H     -2.6252430      1.0873240      1.5262630
H     -3.3489190      4.9628330     -0.2079910
H     -3.9495920      3.1794670      1.4779200
C      2.7734480      1.3137770     -0.1090940
C      1.9756440      1.9559280      0.9140590
C      4.0603460      0.9017780      0.2071870
C      2.5578810      2.2005320      2.2067630
H      1.1757560      2.6389140      0.6349460
C      4.5936230      1.1304130      1.4845790
H      4.6603750      0.3764760     -0.5382100
C      3.8354300      1.7790830      2.4875370
H      1.9548870      2.7211580      2.9518160
H      5.6056280      0.7883210      1.7091070
H      4.2739700      1.9545450      3.4708960
N     -1.5239270     -1.0007920      1.0948080
N      0.9219390     -1.6668820     -0.2027350
N     -1.3657780      1.6488420     -0.0415280
Mn    -0.2019790     -0.0144860     -0.0226740
O      0.7475130      0.5523040      1.2555590
63
Triplet_TS_MnBnTPEN_Oxo_G3.log
63
Final Energy =           -2545.9308078300
C     -3.0583110     -0.0627160      0.4097390
C     -1.8976080     -0.6187130      2.3694450
C     -3.0902110     -0.8115000      3.0605430
C     -4.2981410     -0.6190210      2.3876120
C     -4.2834550     -0.2442930      1.0411560
H     -0.9230060     -0.7509300      2.8428870
H     -3.0637020     -1.1093800      4.1088250
H     -5.2481010     -0.7674140      2.9038660
H     -5.2087740     -0.0980670      0.4831960
C     -2.8932630      0.3638380     -1.0264270
H     -2.8191790      1.4579450     -1.0972670
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H	-3.7449940	0.0537690	-1.6481070
N	-1.6215890	-0.2354680	-1.5258090
C	-1.0414680	0.4419280	-2.7224860
H	-1.5688000	0.1299760	-3.6352930
H	-1.1866670	1.5243920	-2.6174310
C	0.4281450	0.0746510	-2.7968770
H	0.5508090	-1.0097180	-2.9160150
H	0.9101900	0.5520440	-3.6622990
N	1.1208300	0.4798410	-1.5279760
C	-1.8260140	-1.7031910	-1.7765890
H	-1.8803780	-1.8870490	-2.8584420
H	-2.8034100	-1.9922970	-1.3650430
C	-0.7865510	-2.5618470	-1.1221640
C	-0.6685190	-3.9232900	-1.3983340
C	0.2376270	-4.6855790	-0.6637620
H	-1.2896830	-4.3744200	-2.1728190
C	0.8325670	-2.7046510	0.5484810
C	0.9904350	-4.0673810	0.3378810
H	0.3478700	-5.7527580	-0.8632050
H	1.3934790	-2.1875120	1.3253950
H	1.6963670	-4.6273010	0.9511940
C	1.4072760	1.9454320	-1.5284890
H	1.5635580	2.3050460	-2.5556950
H	2.3571950	2.1182070	-0.9996810
C	2.3874510	-0.2847010	-1.3707170
H	3.0585620	-0.0572780	-2.2124840
H	2.1454050	-1.3543320	-1.4425290
C	0.3468660	2.7382680	-0.8258910
C	0.2658840	4.1238640	-0.9513740
C	-1.3360150	2.7321800	0.7887630
C	-0.6526580	4.8207580	-0.1693080
H	0.9259120	4.6423800	-1.6475440
C	-1.4559790	4.1127210	0.7287830
H	-1.9493630	2.1498680	1.4734980
H	-0.7347980	5.9058190	-0.2520430
H	-2.1740680	4.6182380	1.3743960
C	3.1193830	-0.0327840	-0.0765580
C	2.4675710	0.0736400	1.1952250
C	4.5078250	0.0257510	-0.0754890
C	3.2127440	0.0800420	2.4086780
H	1.9191810	1.1460660	1.4582630
C	5.2435980	0.1100680	1.1182340
H	5.0374910	-0.0132170	-1.0290550
C	4.6013920	0.1322960	2.3564650
H	2.6641700	0.0997590	3.3514500
H	6.3330410	0.1491910	1.0693620
H	5.1752120	0.1787160	3.2827370
N	-1.8953570	-0.2490150	1.0791470
N	-0.0236410	-1.9662070	-0.1853070
N	-0.4660240	2.0543890	0.0093270
Mn	-0.2487730	0.0366050	-0.0323970
O	1.0466050	0.0894650	1.3418640

63

TS$_{HT}$

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63
Final Energy =            -2545.9308080900
C        -3.0583770       -0.0608300        0.4096820
C        -1.8981000       -0.6174890        2.3694490
C        -3.0908520       -0.8094380        3.0605250
C        -4.2986350       -0.6161950        2.3875500
C        -4.2836600       -0.2415640        1.0410700
H        -0.9236020       -0.7503410        2.8429280
H        -3.0645700       -1.1072710        4.1088260
H        -5.2487080       -0.7639270        2.9037850
H        -5.2088620       -0.0947670        0.4830680
C        -2.8930190        0.3654860       -1.0265150
H        -2.8181870        1.4595370       -1.0974540
H        -3.7449550        0.0559350       -1.6481730
N        -1.6217400       -0.2347360       -1.5258050
C        -1.0411680        0.4421050       -2.7225770
H        -1.5686960        0.1303940       -3.6353540
H        -1.1856480        1.5246790       -2.6176570
C         0.4282020        0.0738410       -2.7968760
H         0.5501430       -1.0106370       -2.9157460
H         0.9105830        0.5507000       -3.6624040
N         1.1211170        0.4788690       -1.5280540
C        -1.8271370       -1.7023650       -1.7763640
H        -1.8817030       -1.8863290       -2.8581870
H        -2.8046840       -1.9907720       -1.3646950
C        -0.7881820       -2.5616130       -1.1218880
C        -0.6710020       -3.9231690       -1.3978810
C         0.2346940       -4.6859270       -0.6632400
H        -1.2924560       -4.3740350       -2.1722860
C         0.8309250       -2.7052140        0.5487100
C         0.9879340       -4.0680690        0.3382860
H         0.3442590       -5.7532010       -0.8625480
H         1.3922100       -2.1883160        1.3255170
H         1.6935390       -4.6283480        0.9516450
C         1.4084170        1.9442940       -1.5288510
H         1.5647280        2.3036460       -2.5561420
H         2.3585270        2.1166000       -1.0002370
C         2.3872690       -0.2864190       -1.3705900
H         3.0584970       -0.0597380       -2.2124620
H         2.1445290       -1.3559180       -1.4419920
C         0.3486010        2.7378690       -0.8261830
C         0.2685140        4.1235100       -0.9517510
C        -1.3341030        2.7330000        0.7886630
C        -0.6494960        4.8210580       -0.1696470
H         0.9288230        4.6415530       -1.6480090
C        -1.4531840        4.1136110        0.7285810
H        -1.9477350        2.1511470        1.4735380
H        -0.7309350        5.9061670       -0.2524510
H        -2.1708750        4.6196430        1.3742340
C         3.1193540       -0.0344460       -0.0765320
C         2.4675940        0.0723600        1.1952470
C         4.5078050        0.0238000       -0.0755140
C         3.2127990        0.0787390        2.4086780
H         1.9195840        1.1449940        1.4581770
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C          5.2436310         0.1081290         1.1181780
H          5.0374290        -0.0154270        -1.0290920
C          4.6014620         0.1306440         2.3564190
H          2.6642560         0.0987250         3.3514620
H          6.3330810         0.1470260         1.0692710
H          5.1753160         0.1770400         3.2826720
N         -1.8955610        -0.2478610         1.0791310
N         -0.0248630        -1.9663350        -0.1851330
N         -0.4646410         2.0545790         0.0091770
Mn        -0.2487540         0.0366290        -0.0324110
O          1.0466330         0.0887070         1.3418800
65
MnBnTPEN_Hydroperoxo_G1.log
65
Final Energy =        -2620.8380578700
C         -3.2175930        -0.0918030         0.9123140
C         -3.4357770         0.3334430        -1.3748860
C         -4.8145090         0.4783930        -1.2539890
C         -5.4001410         0.3327710         0.0051000
C         -4.5890030         0.0485310         1.1058430
H         -2.9242410         0.4405160        -2.3325740
H         -5.4123240         0.7070020        -2.1367080
H         -6.4781910         0.4466500         0.1317500
H         -5.0087430        -0.0615800         2.1062350
C         -2.2407020        -0.4393690         2.0024090
H         -2.0865040        -1.5277610         2.0251390
H         -2.6155100        -0.1466020         2.9945220
N         -0.9436000         0.2154930         1.6946370
C          0.2153080        -0.4225570         2.3653600
H          0.2759570        -0.1273620         3.4250080
H          0.0791840        -1.5102630         2.3399900
C          1.4672690        -0.0017570         1.6250960
H          1.5942050         1.0849050         1.7077150
H          2.3613550        -0.4617270         2.0697860
N          1.3703910        -0.3348480         0.1705430
C         -1.0226010         1.6767410         1.9925730
H         -0.2843500         1.9400930         2.7643410
H         -2.0036880         1.9054270         2.4332510
C         -0.8256260         2.5466740         0.7828660
C         -0.8419800         3.9395250         0.8872740
C         -0.6815660         4.7064220        -0.2634660
H         -0.9824360         4.4056030         1.8636710
C         -0.4990570         2.6696040        -1.5160880
C         -0.5117480         4.0575470        -1.4899630
H         -0.6910230         5.7963910        -0.2065100
H         -0.3649690         2.1131020        -2.4438270
H         -0.3881110         4.6163550        -2.4180400
C          1.7316420        -1.7535070        -0.0844660
H          2.5755920        -2.0706760         0.5441110
H          2.0519900        -1.8292110        -1.1326630
C          2.2562790         0.5770910        -0.6405550
H          1.8970230         1.5980750        -0.4711070
H          2.0773650         0.3224700        -1.6917070
C          0.5592610        -2.6729390         0.0553540
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C       0.7026850     -4.0387440      0.2947570
C      -1.7353730     -2.9083440     -0.2455620
C      -0.4267580     -4.8551220      0.2521650
H       1.6916900     -4.4499860      0.4996590
C      -1.6665080     -4.2808160     -0.0384910
H      -2.6856640     -2.4234920     -0.4664790
H      -0.3398720     -5.9274890      0.4360710
H      -2.5742270     -4.8816550     -0.0982200
C       3.7290650      0.4862730     -0.3134760
C       4.2966840      1.3223440      0.6612220
C       4.5582850     -0.4311460     -0.9783280
C       5.6527510      1.2269870      0.9825980
H       3.6768150      2.0666110      1.1666950
C       5.9146530     -0.5292150     -0.6589550
H       4.1455280     -1.0686580     -1.7633660
C       6.4639440      0.2960520      0.3269310
H       6.0779000      1.8868810      1.7421330
H       6.5455600     -1.2474360     -1.1873690
H       7.5250230      0.2216920      0.5757170
N      -2.6640340      0.0510940     -0.3128140
N      -0.6474870      1.9311870     -0.3982890
N      -0.6473310     -2.1180410     -0.1798110
Mn     -0.6465950     -0.1056080     -0.3838120
O      -0.4471280     -0.1218550     -2.0953650
O       0.3143800     -1.1540960     -2.7095990
H       0.3826560     -0.8227380     -3.6238960
65
MnBnTPEN_Hydroperoxo_G2.log
65
Final Energy =          -2620.8380554000
C       3.2297440      0.1274090      0.8913700
C       3.4294430     -0.2981190     -1.3974440
C       4.8112790     -0.4236470     -1.2909940
C       5.4082240     -0.2678550     -0.0384400
C       4.6049460      0.0066560      1.0705300
H       2.9092590     -0.4138040     -2.3494660
H       5.4028730     -0.6452340     -2.1796840
H       6.4890570     -0.3664330      0.0768180
H       5.0334950      0.1241190      2.0663670
C       2.2595510      0.4625570      1.9913950
H       2.0904490      1.5487700      2.0149950
H       2.6486530      0.1758740      2.9797530
N       0.9683760     -0.2101340      1.6975720
C      -0.1920410      0.4129240      2.3794280
H      -0.2369150      0.1188070      3.4401450
H      -0.0709070      1.5023580      2.3507750
C      -1.4459340     -0.0274730      1.6535980
H      -1.5555790     -1.1157990      1.7401040
H      -2.3414990      0.4206550      2.1073310
N      -1.3695730      0.3031690      0.1972170
C       1.0695930     -1.6699980      1.9955540
H       0.3458910     -1.9416100      2.7781510
H       2.0595210     -1.8862060      2.4222320
C       0.8667310     -2.5434910      0.7893470
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C        0.8962830       -3.9359980        0.8951690
C        0.7309700       -4.7056290       -0.2530880
H        1.0505100       -4.3996480        1.8706230
C        0.5179420       -2.6720680       -1.5061660
C        0.5431730       -4.0598020       -1.4785820
H        0.7504340       -5.7954040       -0.1950240
H        0.3695190       -2.1176940       -2.4330100
H        0.4150750       -4.6208250       -2.4047230
C       -1.7561960        1.7152900       -0.0570330
H       -2.5978540        2.0203430        0.5806310
H       -2.0913370        1.7838360       -1.1010390
C       -2.2481160       -0.6242800       -0.6041440
H       -1.8923380       -1.6422220       -0.4097370
H       -2.0581990       -0.3914640       -1.6582370
C       -0.5969350        2.6533220        0.0678610
C       -0.7594550        4.0176980        0.3035370
C        1.6914150        2.9233810       -0.2526560
C        0.3568110        4.8512600        0.2492020
H       -1.7528710        4.4145530        0.5152220
C        1.6030160        4.2952710       -0.0494760
H        2.6473090        2.4526220       -0.4798190
H        0.2547970        5.9227600        0.4303670
H        2.5008430        4.9098490       -0.1182800
C       -3.7246620       -0.5202180       -0.2996760
C       -4.3046840       -1.2902780        0.7211030
C       -4.5454390        0.3481620       -1.0366170
C       -5.6653060       -1.1760080        1.0158440
H       -3.6921170       -1.9981370        1.2840440
C       -5.9064870        0.4646250       -0.7444000
H       -4.1203240        0.9318120       -1.8565810
C       -6.4684160       -0.2933110        0.2872500
H       -6.1007020       -1.7840870        1.8119440
H       -6.5306820        1.1440640       -1.3290760
H       -7.5330030       -0.2048630        0.5156170
N        2.6651650       -0.0248560       -0.3276420
N        0.6713430       -1.9312160       -0.3907110
N        0.6163080        2.1165500       -0.1751230
Mn       0.6452220        0.1046760       -0.3774190
O        0.4315830        0.1185310       -2.0873120
O       -0.3560520        1.1356660       -2.6939500
H       -0.4221840        0.8056630       -3.6088790
65
MnBnTPEN_Hydroperoxo_G3.log
65
Final Energy =          -2620.8300248200
C       -2.6445880       -1.7458530        0.6341240
C       -2.4220970       -1.6457030       -1.6860520
C       -3.4201820       -2.5999680       -1.8583380
C       -4.0337620       -3.1492310       -0.7318000
C       -3.6460550       -2.7063080        0.5340850
H       -1.8998910       -1.2099550       -2.5356380
H       -3.7047740       -2.9014390       -2.8667180
H       -4.8170080       -3.9020270       -0.8363410
H       -4.1205800       -3.0871910        1.4388540
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C	-2.1698590	-1.1462060	1.9254060
H	-1.3057670	-1.7092430	2.3071360
H	-2.9557270	-1.1726860	2.6968480
N	-1.7316440	0.2348600	1.6187060
C	-0.9387660	0.8547910	2.7153520
H	-1.5875970	1.4345600	3.3876070
H	-0.5053430	0.0493990	3.3200210
C	0.1419410	1.7397330	2.1277840
H	-0.2885880	2.6155130	1.6292550
H	0.8113800	2.1124330	2.9201160
N	0.9207350	0.9649550	1.1205710
C	-2.9014260	1.0831250	1.2683070
H	-3.3475740	1.5212780	2.1726110
H	-3.6750230	0.4501490	0.8093710
C	-2.5240790	2.1341670	0.2703860
C	-3.2229060	3.3323810	0.1353720
C	-2.8613340	4.2132660	-0.8837170
H	-4.0393360	3.5627190	0.8208760
C	-1.1588270	2.6539750	-1.5345750
C	-1.8144690	3.8632170	-1.7385320
H	-3.3907500	5.1595020	-1.0094300
H	-0.3414930	2.3333390	-2.1806410
H	-1.5001090	4.5162520	-2.5531050
C	1.7395320	-0.0685010	1.8126280
H	1.3260850	-0.2482140	2.8133140
H	2.7649710	0.2848450	1.9705960
C	1.7953320	1.9305320	0.3247000
H	2.0018560	2.7840930	0.9858630
H	1.1934360	2.3064100	-0.5088060
C	1.7280030	-1.3683590	1.0746990
C	2.7312250	-2.3203950	1.2567210
C	0.5409870	-2.7976260	-0.3130140
C	2.6111090	-3.5579010	0.6310380
H	3.5909770	-2.0814170	1.8837550
C	1.4871960	-3.8026000	-0.1614010
H	-0.3254480	-2.9512750	-0.9506910
H	3.3822820	-4.3199960	0.7573090
H	1.3452870	-4.7552730	-0.6723170
C	3.1140940	1.3761010	-0.1555830
C	3.2049990	0.4163350	-1.1755380
C	4.2971640	1.8284450	0.4511570
C	4.4485210	-0.0857160	-1.5661390
H	2.3097310	0.0444420	-1.6661650
C	5.5418450	1.3317150	0.0562790
H	4.2418040	2.5769070	1.2457450
C	5.6198610	0.3676880	-0.9525520
H	4.4995660	-0.8373440	-2.3571310
H	6.4503150	1.6972220	0.5400750
H	6.5905310	-0.0271010	-1.2612440
N	-2.0349940	-1.2431680	-0.4626270
N	-1.4992080	1.8114270	-0.5422980
N	0.6541600	-1.5985340	0.2913010
Mn	-0.5149040	0.0462210	-0.1370970
O	0.0255310	0.1419700	-1.7790720

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O         0.4776240        -0.9870880        -2.5206600
H         0.5200540        -0.6138530        -3.4201980
68
MnBnTPEN_MeCN_G1.log
68
Final Energy =          -2602.4603401200
C         3.0256980        -0.2386370        -1.3636330
C         3.4299930        -0.2342910         0.9439350
C         4.7873890        -0.4532460         0.7386240
C         5.2599160        -0.5949090        -0.5675190
C         4.3677110        -0.4749200        -1.6353560
H         3.0189390        -0.1230590         1.9469100
H         5.4547030        -0.5135070         1.5983230
H         6.3189080        -0.7792860        -0.7553770
H         4.7048450        -0.5459880        -2.6696760
C         1.9571900        -0.0162370        -2.3869750
H         1.4477610        -0.9625360        -2.6202320
H         2.3653690         0.3849700        -3.3265830
N         0.9762500         0.9162680        -1.7698520
C        -0.2887770         1.0207650        -2.5645010
H        -0.3072870         1.9524920        -3.1441060
H        -0.3121710         0.2019740        -3.2924280
C        -1.4677850         0.9617770        -1.6207610
H        -1.5667630         1.8903040        -1.0475140
H        -2.4083380         0.8107480        -2.1697340
N        -1.2354700        -0.1571320        -0.6662330
C         1.5917390         2.2620050        -1.5856360
H         1.4821760         2.8667760        -2.4958970
H         2.6713720         2.1463340        -1.4102320
C         1.0025790         2.9338610        -0.3894920
C         0.9529650         4.3137410        -0.2334050
C         0.4645560         4.8417780         0.9630260
H         1.2958360         4.9611410        -1.0407370
C         0.1169190         2.6032820         1.7476280
C         0.0453570         3.9706900         1.9712110
H         0.4126110         5.9224210         1.1062190
H        -0.2031620         1.8981930         2.5119330
H        -0.3381070         4.3395830         2.9224550
C        -1.3729860        -1.4643330        -1.3558320
H        -1.0661100        -1.3556680        -2.4031550
H        -2.4264530        -1.7718810        -1.3793940
C        -2.1577160        -0.0889630         0.5401100
H        -1.8867990         0.8141600         1.1004380
H        -1.9275270        -0.9634750         1.1580160
C        -0.4966820        -2.4736570        -0.6984670
C        -0.7324990        -3.8450480        -0.7769110
C         1.4504210        -2.8101160         0.5116920
C         0.1787010        -4.7198350        -0.1897620
H        -1.6202280        -4.2106330        -1.2937660
C         1.2914050        -4.1889360         0.4653120
H         2.3003530        -2.3799720         1.0362020
H         0.0199340        -5.7984690        -0.2362330
H         2.0305940        -4.8287370         0.9475810
C        -3.6281150        -0.0580540         0.2025030
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C	-4.2776290	1.1589210	-0.0560040
C	-4.3670070	-1.2511120	0.1556040
C	-5.6342220	1.1797830	-0.3849730
H	-3.7258080	2.0989590	0.0126990
C	-5.7245650	-1.2296460	-0.1733210
H	-3.8861330	-2.2025490	0.3962570
C	-6.3579980	-0.0150900	-0.4510890
H	-6.1290020	2.1329020	-0.5830080
H	-6.2889920	-2.1638900	-0.2047020
H	-7.4194470	0.0020890	-0.7078160
N	2.5748810	-0.1446280	-0.0929280
N	0.5754180	2.0916260	0.5826370
N	0.5777480	-1.9624710	-0.0657060
Mn	0.6211270	0.1384150	0.1671420
N	0.4605230	-0.4006250	2.0681010
C	0.3727820	-0.7758970	3.1580340
C	0.2573430	-1.2457750	4.5178870
H	0.6963120	-2.2515680	4.5948520
H	0.7859460	-0.5547470	5.1912220
H	-0.8070670	-1.2861440	4.7952290
68			

MnBnTPEN_MeCN_G2.log
68
Final Energy =   -2602.4562737100

C	2.2885570	-1.9808240	-0.9268960
C	2.2506840	-1.9328910	1.4074470
C	3.0645160	-3.0580490	1.4764900
C	3.4730350	-3.6729820	0.2923490
C	3.0920470	-3.1148140	-0.9291890
H	1.9207150	-1.4237070	2.3100320
H	3.3678460	-3.4371450	2.4524370
H	4.1026000	-4.5638880	0.3180350
H	3.4256510	-3.5383880	-1.8768170
C	1.8754600	-1.2190270	-2.1447880
H	0.9049310	-1.5782520	-2.5156210
H	2.6051630	-1.3259190	-2.9617050
N	1.7338570	0.1994500	-1.7261010
C	1.0878330	1.0326420	-2.7923360
H	1.8293260	1.6721260	-3.2871620
H	0.6864520	0.3662220	-3.5643330
C	0.0091320	1.8673840	-2.1479070
H	0.4398930	2.6897180	-1.5657880
H	-0.6733540	2.3062100	-2.8918170
N	-0.7509330	0.9870710	-1.2155030
C	3.0619230	0.7648530	-1.3500950
H	3.5885960	1.1367490	-2.2389720
H	3.6859400	-0.0320680	-0.9216600
C	2.8876720	1.8258490	-0.3132940
C	3.7824180	2.8751170	-0.1359460
C	3.5725480	3.7732140	0.9114800
H	4.6305180	2.9814100	-0.8127950
C	1.6157010	2.5258360	1.5126080
C	2.4707870	3.5931300	1.7502990
H	4.2601840	4.6060560	1.0681810

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H         0.7467960        2.3617910        2.1473770
H         2.2668210        4.2698300        2.5800910
C        -1.5846150        0.0194400       -1.9687990
H        -1.0676650       -0.2363910       -2.9017830
H        -2.5415700        0.4727290       -2.2546200
C        -1.5215950        1.8225360       -0.1957100
H        -1.4289380        2.8675810       -0.5158390
H        -0.9835280        1.7590660        0.7631380
C        -1.7690790       -1.2122920       -1.1524240
C        -2.8147930       -2.1096240       -1.3594550
C        -0.9000060       -2.5109810        0.5594870
C        -2.8871410       -3.2502010       -0.5652140
H        -3.5619630       -1.8976290       -2.1245450
C        -1.9114280       -3.4505450        0.4149090
H        -0.1367710       -2.6418430        1.3231480
H        -3.6974780       -3.9685980       -0.6995200
H        -1.9295280       -4.3221500        1.0693490
C        -2.9680080        1.4602670       -0.0010590
C        -3.3699000        0.4910880        0.9286930
C        -3.9404460        2.1000230       -0.7861710
C        -4.7182880        0.1554330        1.0625400
H        -2.6314190       -0.0153950        1.5474720
C        -5.2886190        1.7619500       -0.6553430
H        -3.6376900        2.8639620       -1.5068010
C        -5.6790070        0.7862390        0.2675180
H        -5.0163830       -0.6033720        1.7885470
H        -6.0356840        2.2641410       -1.2733400
H        -6.7336130        0.5217650        0.3702640
N         1.8529690       -1.4246980        0.2252910
N         1.8148780        1.6600420        0.4954820
N        -0.8221050       -1.4112410       -0.2149640
Mn        0.5792670        0.1318640        0.0587240
N        -0.0377490       -0.0028180        1.9606630
C        -0.3956860       -0.1078350        3.0550370
C        -0.8606020       -0.2461690        4.4138820
H        -1.0865820       -1.3041040        4.6144820
H        -0.0834550        0.1086550        5.1068240
H        -1.7725030        0.3569880        4.5428630
68
MnBnTPEN_MeCN_G3.log
68
Final Energy =         -2602.4603400800
C        -3.0256470        0.2387990       -1.3637590
C        -3.4301050        0.2347480        0.9437680
C        -4.7874550        0.4538470        0.7383380
C        -5.2598750        0.5954440       -0.5678530
C        -4.3676050        0.4752360       -1.6356080
H        -3.0191600        0.1235550        1.9467950
H        -5.4548190        0.5142710        1.5979880
H        -6.3188290        0.7799380       -0.7558030
H        -4.7046380        0.5462500       -2.6699640
C        -1.9571120        0.0161940       -2.3870320
H        -1.4476160        0.9624380       -2.6203760
H        -2.3652990       -0.3850630       -3.3266150
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N	-0.9762830	-0.9163480	-1.7697920
C	0.2887780	-1.0210500	-2.5643570
H	0.3072500	-1.9528500	-3.1438470
H	0.3122950	-0.2023480	-3.2923800
C	1.4677570	-0.9620030	-1.6205900
H	1.5667540	-1.8904720	-1.0472580
H	2.4083090	-0.8109910	-2.1695690
N	1.2354060	0.1569920	-0.6661530
C	-1.5919290	-2.2620000	-1.5855250
H	-1.4826150	-2.8667300	-2.4958470
H	-2.6715130	-2.1461850	-1.4098920
C	-1.0026010	-2.9339510	-0.3895160
C	-0.9530050	-4.3138440	-0.2335250
C	-0.4643780	-4.8419630	0.9627790
H	-1.2960600	-4.9611750	-1.0408340
C	-0.1165350	-2.6035190	1.7474520
C	-0.0449580	-3.9709430	1.9709320
H	-0.4124200	-5.9226150	1.1059020
H	0.2037070	-1.8984940	2.5117520
H	0.3386880	-4.3399070	2.9220750
C	1.3728570	1.4641390	-1.3558550
H	1.0659390	1.3554310	-2.4031580
H	2.4263180	1.7716960	-1.3795110
C	2.1576910	0.0889620	0.5401860
H	1.8869150	-0.8141960	1.1005170
H	1.9274050	0.9634480	1.1580910
C	0.4966540	2.4735180	-0.6984540
C	0.7324930	3.8448960	-0.7770450
C	-1.4501340	2.8101140	0.5121580
C	-0.1785420	4.7197480	-0.1897400
H	1.6201150	4.2104310	-1.2941180
C	-1.2910910	4.1889240	0.4656570
H	-2.2999370	2.3800400	1.0369260
H	-0.0197590	5.7983740	-0.2363310
H	-2.0301390	4.8287750	0.9480760
C	3.6280790	0.0582470	0.2025140
C	4.2777300	-1.1586470	-0.0560260
C	4.3668200	1.2513970	0.1555480
C	5.6343020	-1.1793410	-0.3850950
H	3.7260430	-2.0987580	0.0127330
C	5.7243560	1.2301000	-0.1734800
H	3.8858490	2.2027820	0.3962130
C	6.3579240	0.0156220	-0.4512830
H	6.1291850	-2.1324020	-0.5831530
H	6.2886520	2.1644220	-0.2049170
H	7.4193530	-0.0014310	-0.7081010
N	-2.5749170	0.1448730	-0.0930190
N	-0.5752380	-2.0917820	0.5825790
N	-0.5776420	1.9624010	-0.0654140
Mn	-0.6212280	-0.1384980	0.1672180
N	-0.4606760	0.4002900	2.0682830
C	-0.3730120	0.7754050	3.1582740
C	-0.2577040	1.2450840	4.5182070
H	-0.6965620	2.2509220	4.5952310

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H          -0.7864700          0.5540220          5.1913810
H           0.8066690          1.2853040          4.7957100
63
MnBnTPEN_Oxo_G1.log
63
Final Energy =              -2544.8799232900
C          -3.0706490         -0.3218430         -0.3027620
C          -2.1253220          0.4949580         -2.2934790
C          -3.3793410          0.5962450         -2.8827480
C          -4.5075480          0.2286040         -2.1483290
C          -4.3493680         -0.2331130         -0.8406220
H          -1.2211310          0.7650540         -2.8374640
H          -3.4565870          0.9629060         -3.9064230
H          -5.5038440          0.3055970         -2.5864990
H          -5.2063710         -0.5207530         -0.2313450
C          -2.7716320         -0.8422850          1.0710500
H          -2.5728640         -1.9221330          1.0322160
H          -3.6209400         -0.7010460          1.7538960
N          -1.5587620         -0.1425500          1.5563390
C          -0.8340020         -0.8716710          2.6276530
H          -1.3372400         -0.7484100          3.5989160
H          -0.8381860         -1.9438900          2.4015910
C           0.5592000         -0.2961920          2.6762140
H           0.5328060          0.7659450          2.9512400
H           1.1785230         -0.8092110          3.4243720
N           1.2247290         -0.3955310          1.3302860
C          -1.9147780          1.2345460          2.0101100
H          -1.7494890          1.3317170          3.0920940
H          -2.9910450          1.4009300          1.8573670
C          -1.1800510          2.2962910          1.2602680
C          -1.3376050          3.6468150          1.5775420
C          -0.7498920          4.6107800          0.7661140
H          -1.9368650          3.9236450          2.4455390
C           0.0988760          2.8427600         -0.6117520
C          -0.0376410          4.1979710         -0.3637160
H          -0.8619520          5.6711040          0.9978220
H           0.6369870          2.4863540         -1.4867900
H           0.4148240          4.9127640         -1.0512290
C           1.7174250         -1.7821930          1.0933820
H           2.1608410         -2.1954260          2.0097560
H           2.5128050         -1.7335790          0.3373530
C           2.3987780          0.5940980          1.3474400
H           2.9403200          0.3694950          2.2794430
H           1.9541140          1.5891120          1.4534640
C           0.6677820         -2.6710820          0.5240620
C           0.7254510         -4.0581540          0.6150570
C          -1.1461740         -2.7892200         -0.9549920
C          -0.1894710         -4.8205190         -0.1087150
H           1.4910130         -4.5236690          1.2355070
C          -1.1245390         -4.1737760         -0.9230130
H          -1.8604640         -2.2580220         -1.5778530
H          -0.1660800         -5.9098590         -0.0495260
H          -1.8385520         -4.7309930         -1.5290650
C           3.3501470          0.5384580          0.1899340
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C      4.3873910     -0.4140110      0.1440110
C      3.2681260      1.4901910     -0.8455370
C      5.2589220     -0.4591560     -0.9418320
H      4.5284760     -1.1132220      0.9707590
C      4.1404620      1.4461110     -1.9345700
H      2.5464130      2.3004330     -0.7721530
C      5.1268420      0.4611700     -1.9928640
H      6.0544670     -1.2062150     -0.9665680
H      4.0562720      2.1923700     -2.7265400
H      5.8130230      0.4214290     -2.8413270
N     -1.9864900      0.0410530     -1.0308480
N     -0.4312850      1.9082870      0.2133030
N     -0.2815720     -2.0544230     -0.2179390
Mn    -0.1811050     -0.0745070     -0.1727660
O      0.7767090      0.2009630     -1.3081010
63
MnBnTPEN_Oxo_G2.log
63
Final Energy =          -2544.8799231200
C     -3.0704890     -0.3216430     -0.3030360
C     -2.1248900      0.4951830     -2.2936100
C     -3.3788450      0.5966940     -2.8829650
C     -4.5071660      0.2291290     -2.1486760
C     -4.3491600     -0.2327210     -0.8409950
H     -1.2206090      0.7652350     -2.8374690
H     -3.4559670      0.9634730     -3.9066070
H     -5.5034130      0.3062640     -2.5869340
H     -5.2062500     -0.5203120     -0.2318180
C     -2.7716580     -0.8422170      1.0707680
H     -2.5729290     -1.9220660      1.0318730
H     -3.6210350     -0.7009830      1.7535290
N     -1.5588050     -0.1425750      1.5562820
C     -0.8341890     -0.8718670      2.6276040
H     -1.3375350     -0.7486230      3.5988120
H     -0.8384320     -1.9440650      2.4014560
C      0.5590480     -0.2965160      2.6763520
H      0.5327530      0.7656090      2.9514530
H      1.1782290     -0.8096960      3.4245200
N      1.2246480     -0.3958900      1.3304650
C     -1.9147730      1.2344920      2.0101710
H     -1.7494340      1.3315390      3.0921560
H     -2.9910370      1.4009130      1.8574300
C     -1.1800100      2.2962690      1.2603980
C     -1.3376550      3.6467810      1.5776690
C     -0.7498760      4.6107760      0.7663210
H     -1.9370350      3.9235900      2.4455890
C      0.0992080      2.8428000     -0.6114020
C     -0.0374270      4.1980040     -0.3633890
H     -0.8620370      5.6710960      0.9980000
H      0.6376050      2.4864000     -1.4862620
H      0.4151020      4.9128270     -1.0508300
C      1.7172600     -1.7825660      1.0935630
H      2.1605370     -2.1958580      2.0099690
H      2.5127200     -1.7339860      0.3376260
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C       2.3987860       0.5936360       1.3476700
H       2.9404240       0.3687340       2.2795530
H       1.9541850       1.5886450       1.4540440
C       0.6676390      -2.6713490       0.5240560
C       0.7252120      -4.0584180       0.6149310
C      -1.1461820      -2.7892310      -0.9551660
C      -0.1897160      -4.8206670      -0.1089650
H       1.4907090      -4.5240610       1.2353690
C      -1.1246700      -4.1737890      -0.9232790
H      -1.8603500      -2.2579620      -1.5781040
H      -0.1664170      -5.9100130      -0.0498390
H      -1.8386920      -4.7308870      -1.5294310
C       3.3499960       0.5382340       0.1900170
C       3.2681790       1.4906050      -0.8449040
C       4.3869290      -0.4145390       0.1434370
C       4.1403720       1.4468510      -1.9340560
H       2.5467590       2.3010560      -0.7709520
C       5.2582900      -0.4593810      -0.9425570
H       4.5279650      -1.1141860       0.9698180
C       5.1263840       0.4615760      -1.9930520
H       4.0563510       2.1935970      -2.7255860
H       6.0536040      -1.2066670      -0.9678090
H       5.8124260       0.4220400      -2.8416360
N      -1.9862230       0.0411200      -1.0310170
N      -0.4310800       1.9082930       0.2135350
N      -0.2816030      -2.0545280      -0.2179830
Mn     -0.1809840      -0.0745730      -0.1726190
O       0.7767840       0.2013750      -1.3078590
63
MnBnTPEN_Oxo_G3.log
63
Final Energy =          -2544.8814804500
C       3.2116700       0.0593970       0.7888900
C       3.3642790      -0.5886750      -1.4672650
C       4.7396030      -0.7490260      -1.3573690
C       5.3602270      -0.4904740      -0.1346170
C       4.5836890      -0.0882580       0.9536750
H       2.8460990      -0.7745400      -2.4069620
H       5.3065120      -1.0733790      -2.2301950
H       6.4389720      -0.6113300      -0.0241530
H       5.0279380       0.1034180       1.9306570
C       2.2696510       0.4880080       1.8739120
H       2.1548170       1.5799810       1.8814580
H       2.6387320       0.2008380       2.8684730
N       0.9611050      -0.1456100       1.5782770
C      -0.1912260       0.5280460       2.2303090
H      -0.2569180       0.2542650       3.2938580
H      -0.0435070       1.6130510       2.1865350
C      -1.4335430       0.0948480       1.4939520
H      -1.5869240      -0.9853830       1.5981330
H      -2.3279380       0.5916540       1.8901720
N      -1.3042280       0.3907480       0.0263680
C       1.0252620      -1.5927410       1.9426000
H       0.4426100      -1.7812750       2.8553590
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H       2.0637490      -1.8556080       2.1898040
C       0.5841290      -2.4834840       0.8277890
C       0.3852650      -3.8512890       1.0187450
C       0.0693710      -4.6522520      -0.0741000
H       0.4903130      -4.2714010       2.0194700
C       0.1528680      -2.6975310      -1.4611920
C      -0.0382960      -4.0633820      -1.3372680
H      -0.0878720      -5.7242180       0.0550380
H       0.0611310      -2.2020540      -2.4269300
H      -0.2767760      -4.6492080      -2.2251130
C      -1.5667530       1.8330590      -0.2610960
H      -2.3941710       2.2030990       0.3571300
H      -1.8807260       1.9191090      -1.3119480
C      -2.2731920      -0.4836080      -0.7728500
H      -1.9998280      -1.5208820      -0.5644100
H      -2.0775780      -0.2740520      -1.8312240
C      -0.3398430       2.6685140      -0.1067170
C      -0.3882580       4.0427660       0.0995650
C       1.9862140       2.7416150      -0.4011900
C       0.7966900       4.7760970       0.0487000
H      -1.3486760       4.5247950       0.2827930
C       1.9977980       4.1161900      -0.2276370
H       2.9032910       2.1991060      -0.6153660
H       0.7820070       5.8550150       0.2111950
H       2.9424970       4.6540080      -0.3050190
C      -3.7181390      -0.2467120      -0.4267640
C      -4.3421600      -1.0111590       0.5741640
C      -4.4696470       0.7231630      -1.1122940
C      -5.6809750      -0.7936680       0.8997200
H      -3.7838600      -1.7936250       1.0925650
C      -5.8090800       0.9396530      -0.7877390
H      -4.0143990       1.3002430      -1.9198130
C      -6.4148140       0.1872460       0.2240630
H      -6.1552240      -1.3965890       1.6766230
H      -6.3839110       1.6916680      -1.3318460
H      -7.4632790       0.3572520       0.4781670
N       2.6287210      -0.1811610      -0.4116110
N       0.4489560      -1.9242090      -0.3882100
N       0.8382580       2.0326860      -0.3140040
Mn      0.6548740       0.0809200      -0.5908110
O       0.4295840       0.0247290      -2.0784770
64
MnBnTPEN_Peroxide_Mn3_G1.log
64
Final Energy =          -2620.3804956900
C      -3.3291550       0.0053270       0.8788960
C      -3.6136230       0.4242400      -1.3856390
C      -4.9895970       0.5724820      -1.2253670
C      -5.5425730       0.4331800       0.0480660
C      -4.6942180       0.1453970       1.1187630
H      -3.1290500       0.4995020      -2.3589790
H      -5.6117800       0.7946260      -2.0933950
H      -6.6162280       0.5493180       0.2078640
H      -5.0793580       0.0300030       2.1327450
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C      -2.3364920     -0.3537430      1.9445270
H      -2.2026850     -1.4450220      1.9619820
H      -2.6859410     -0.0552440      2.9463280
N      -1.0407370      0.2660810      1.6041290
C       0.0746270     -0.4032720      2.3112870
H       0.0886160     -0.1235360      3.3783330
H      -0.0932230     -1.4863880      2.2639760
C       1.3820650     -0.0314960      1.6519530
H       1.5694510      1.0420170      1.7855120
H       2.2178800     -0.5643390      2.1330440
N       1.3332950     -0.3033610      0.1963170
C      -1.0890900      1.7262860      1.8919990
H      -0.6478910      1.9425860      2.8774050
H      -2.1455960      2.0279340      1.9564220
C      -0.4597430      2.5663540      0.8151890
C      -0.0492930      3.8807790      1.0435560
C       0.4177880      4.6376440     -0.0317130
H      -0.1046920      4.3005840      2.0491190
C       0.0459750      2.7335560     -1.4463110
C       0.4551340      4.0557120     -1.3013390
H       0.7460300      5.6678300      0.1198890
H       0.0525610      2.2062570     -2.4006710
H       0.8081960      4.6127490     -2.1702720
C       1.5680360     -1.7310710     -0.1181510
H       2.3910560     -2.1446600      0.4850370
H       1.8820890     -1.7796750     -1.1700470
C       2.3260370      0.5500310     -0.5321040
H       2.1399510      1.5849000     -0.2242930
H       2.0674990      0.4622320     -1.5940390
C       0.3452420     -2.6010870     -0.0134890
C       0.4498030     -3.9665060      0.2580840
C      -1.9373930     -2.7946250     -0.3781060
C      -0.6930510     -4.7636890      0.1940120
H       1.4221840     -4.3941940      0.5069760
C      -1.9084460     -4.1669220     -0.1459650
H      -2.8693850     -2.2916780     -0.6352830
H      -0.6342260     -5.8339940      0.4007880
H      -2.8276730     -4.7485980     -0.2252110
C       3.7769650      0.2015720     -0.2869520
C       4.4683050      0.7178920      0.8211790
C       4.4646970     -0.6491370     -1.1666920
C       5.8019120      0.3743610      1.0573860
H       3.9640980      1.4081940      1.5011460
C       5.7985270     -0.9950720     -0.9349050
H       3.9524850     -1.0393280     -2.0497650
C       6.4693840     -0.4881480      0.1821510
H       6.3235560      0.7874650      1.9239180
H       6.3167940     -1.6576820     -1.6320320
H       7.5127430     -0.7559570      0.3646230
N      -2.7975390      0.1502700     -0.3539290
N      -0.3923490      2.0052120     -0.4050140
N      -0.8398750     -2.0237720     -0.2976730
Mn     -0.7254120      0.0086530     -0.5168200
O      -1.0654540      0.3018760     -2.3524380
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O          0.1001220        -0.4210650        -2.1762250
64
MnBnTPEN_Peroxide_Mn3_G2.log
64
Final Energy =              -2620.3804957400
C          3.3291610        -0.0055120         0.8786200
C          3.6136420        -0.4245380        -1.3858760
C          4.9896570        -0.5722520        -1.2256890
C          5.5426980        -0.4326050         0.0476970
C          4.6943120        -0.1450410         1.1184100
H          3.1289710        -0.5000360        -2.3591550
H          5.6118580        -0.7942290        -2.0937480
H          6.6164130        -0.5483160         0.2073910
H          5.0794380        -0.0293790         2.1323670
C          2.3365760         0.3533640         1.9444140
H          2.2027780         1.4446420         1.9621060
H          2.6861930         0.0546920         2.9461040
N          1.0407930        -0.2664280         1.6041160
C         -0.0745630         0.4028390         2.3113750
H         -0.0886430         0.1228490         3.3783530
H          0.0933550         1.4859540         2.2643100
C         -1.3820240         0.0312830         1.6519430
H         -1.5695040        -1.0422300         1.7853500
H         -2.2177580         0.5641440         2.1331620
N         -1.3332830         0.3033780         0.1963510
C          1.0892290        -1.7266500         1.8919230
H          0.6484450        -1.9429570         2.8775140
H          2.1457660        -2.0282900         1.9558710
C          0.4594430        -2.5666350         0.8153210
C          0.0486910        -3.8809520         1.0437780
C         -0.4187980        -4.6376880        -0.0314010
H          0.1041600        -4.3007700         2.0493300
C         -0.0467410        -2.7337320        -1.4460930
C         -0.4562330        -4.0557810        -1.3010320
H         -0.7472770        -5.6677890         0.1202810
H         -0.0532810        -2.2064070        -2.4004440
H         -0.8096030        -4.6127530        -2.1698800
C         -1.5677390         1.7311650        -0.1178580
H         -2.3906520         2.1448270         0.4854370
H         -1.8818620         1.7800210        -1.1697190
C         -2.3261460        -0.5496520        -0.5322680
H         -2.1402730        -1.5846420        -0.2247410
H         -2.0675760        -0.4615920        -1.5941830
C         -0.3447810         2.6009590        -0.0131790
C         -0.4491470         3.9663840         0.2584450
C          1.9378620         2.7942280        -0.3779020
C          0.6937980         4.7634320         0.1943050
H         -1.4214520         4.3941950         0.5074250
C          1.9090970         4.1665310        -0.1457660
H          2.8697930         2.2911760        -0.6350990
H          0.6351200         5.8337400         0.4011080
H          2.8283730         4.7481170        -0.2250990
C         -3.7770310        -0.2010020        -0.2871070
C         -4.4684650        -0.7171970         0.8210280
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C      -4.4646150       0.6498060      -1.1668630
C      -5.8020040      -0.3734050       1.0572320
H      -3.9644170      -1.4076190       1.5009880
C      -5.7983800       0.9959950      -0.9350790
H      -3.9523050       1.0398720      -2.0499370
C      -6.4693180       0.4892240       0.1819930
H      -6.3237230      -0.7864020       1.9237700
H      -6.3165420       1.6586800      -1.6322140
H      -7.5126230       0.7572400       0.3644690
N       2.7974990      -0.1507790      -0.3541310
N       0.3919650      -2.0055210      -0.4048720
N       0.8402620       2.0235070      -0.2974150
Mn      0.7254100      -0.0089230      -0.5168790
O       1.0650840      -0.3024650      -2.3524740
O      -0.0998520       0.4214470      -2.1762400
64
MnBnTPEN_Peroxide_Mn3_G3.log
64
Final Energy =             -2620.3714901800
C      -2.2981100      -2.0606370       0.8600820
C      -2.2337450      -2.2432450      -1.4511940
C      -2.9991440      -3.4071370      -1.4200890
C      -3.4158990      -3.9111450      -0.1882880
C      -3.0645990      -3.2176670       0.9714650
H      -1.8663750      -1.8170550      -2.3847290
H      -3.2597400      -3.9036470      -2.3556490
H      -4.0158720      -4.8212100      -0.1293230
H      -3.3860030      -3.5592570       1.9564100
C      -1.8879930      -1.2255950       2.0369610
H      -0.9120120      -1.5695210       2.4102920
H      -2.6110490      -1.3181090       2.8648880
N      -1.7449190       0.1662820       1.5711250
C      -1.0937600       1.0499410       2.5770890
H      -1.8396010       1.6922380       3.0673540
H      -0.6689170       0.4248550       3.3716190
C      -0.0259590       1.9143780       1.9300260
H      -0.4807130       2.7215970       1.3429140
H       0.5924530       2.3873340       2.7138780
N       0.8103490       1.1114830       1.0121050
C      -3.0657460       0.7224570       1.1852050
H      -3.6265010       1.0557030       2.0720270
H      -3.6598550      -0.0705310       0.7090160
C      -2.8832040       1.8257790       0.1887460
C      -3.7544100       2.9065930       0.0601710
C      -3.5263700       3.8320590      -0.9599630
H      -4.5954070       3.0126820       0.7470020
C      -1.6072800       2.5397050      -1.6124720
C      -2.4364030       3.6414190      -1.8120110
H      -4.1898050       4.6900690      -1.0859390
H      -0.7290780       2.3335710      -2.2257600
H      -2.2219260       4.3400380      -2.6220480
C       1.5403520       0.0607420       1.7640000
H       0.9091330      -0.2883910       2.5896820
H       2.4572490       0.4490020       2.2268770
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C      1.7491160      2.0507170      0.2769570
H      1.8961900      2.9304430      0.9219850
H      1.2255080      2.3691380     -0.6310950
C      1.8290810     -1.1115140      0.8787220
C      2.9777950     -1.8933230      0.9939280
C      1.0617460     -2.3751320     -0.9034640
C      3.1541940     -2.9625260      0.1177890
H      3.7300800     -1.6412110      1.7420440
C      2.1816150     -3.2004790     -0.8564170
H      0.2957300     -2.4974350     -1.6679470
H      4.0470370     -3.5878000      0.1791110
H      2.2884070     -4.0090860     -1.5808070
C      3.1128250      1.4910590     -0.0602070
C      3.3400440      0.7235840     -1.2133470
C      4.1907370      1.7359910      0.8068570
C      4.6067990      0.1980080     -1.4771440
H      2.5001930      0.5169750     -1.8770230
C      5.4568010      1.2048760      0.5482310
H      4.0364390      2.3486330      1.6992560
C      5.6669030      0.4285000     -0.5956350
H      4.7640840     -0.4052430     -2.3745980
H      6.2804840      1.4016620      1.2385160
H      6.6553010      0.0102340     -0.8009290
N     -1.8805240     -1.5865570     -0.3334080
N     -1.8263510      1.6566390     -0.6243040
N      0.8776010     -1.3666920     -0.0375170
Mn    -0.5950120      0.0430570     -0.2946230
O      0.4511970      0.5741970     -1.7840340
O     -0.6818920     -0.1297750     -2.1838980
64
MnBnTPEN_Peroxide_Mn4_G2.log
64
Final Energy =        -2620.2195639800
C      3.2551630      0.0875040      0.9732850
C      3.5554240     -0.6235500     -1.2267470
C      4.9248390     -0.7673140     -1.0291410
C      5.4661390     -0.4580230      0.2190330
C      4.6145860     -0.0332800      1.2403150
H      3.0871570     -0.8565650     -2.1819390
H      5.5494340     -1.1220600     -1.8492810
H      6.5369950     -0.5613740      0.4024070
H      4.9915870      0.1920210      2.2381940
C      2.2288740      0.5060120      1.9759450
H      2.0852810      1.5947870      1.9496870
H      2.5170950      0.2407920      3.0040530
N      0.9526430     -0.1512240      1.5946440
C     -0.1963770      0.4985460      2.2809010
H     -0.2149420      0.2226090      3.3462460
H     -0.0585070      1.5848140      2.2284110
C     -1.4570090      0.0645400      1.5859260
H     -1.6101640     -1.0127610      1.7236090
H     -2.3369260      0.5709910      2.0058180
N     -1.3526590      0.3219200      0.1178100
C      1.0280930     -1.6205500      1.8980330
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H        0.4457240      -1.8459960       2.8023860
H        2.0705090      -1.8741080       2.1388640
C        0.6007350      -2.4928680       0.7513980
C        0.3887370      -3.8632510       0.9047690
C        0.0846080      -4.6260370      -0.2216350
H        0.4706370      -4.3187230       1.8923570
C        0.1933560      -2.6299070      -1.5464010
C       -0.0043060      -4.0016330      -1.4699610
H       -0.0817360      -5.7006200      -0.1272660
H        0.1042630      -2.0763580      -2.4813040
H       -0.2359710      -4.5663920      -2.3731860
C       -1.6596770       1.7408380      -0.2188140
H       -2.5015960       2.1078110       0.3838580
H       -1.9720570       1.7654550      -1.2709740
C       -2.3123860      -0.5912290      -0.6141680
H       -2.0286860      -1.6158260      -0.3546810
H       -2.1314440      -0.4506870      -1.6837460
C       -0.4740750       2.6525330      -0.1110400
C       -0.6111950       4.0294060       0.0632560
C        1.8313270       2.8614200      -0.3861870
C        0.5250800       4.8347030      -0.0015610
H       -1.5996060       4.4571120       0.2343200
C        1.7666650       4.2420100      -0.2456320
H        2.7788070       2.3563930      -0.5723320
H        0.4422170       5.9149920       0.1299480
H        2.6779350       4.8355170      -0.3212130
C       -3.7689380      -0.3630490      -0.2811640
C       -4.3807780      -1.0607280       0.7726650
C       -4.5415160       0.5384720      -1.0305550
C       -5.7235690      -0.8417640       1.0886020
H       -3.8085280      -1.7942900       1.3452200
C       -5.8843610       0.7596300      -0.7165940
H       -4.0953140       1.0654600      -1.8769320
C       -6.4767510       0.0744460       0.3484160
H       -6.1842760      -1.3941810       1.9104850
H       -6.4711400       1.4635890      -1.3107700
H       -7.5274140       0.2454100       0.5935630
N        2.7440820      -0.1861200      -0.2479910
N        0.4850140      -1.9033660      -0.4515970
N        0.7341340       2.0884800      -0.2994330
Mn       0.7068040       0.0772340      -0.4667370
O        1.2125410       0.2105070      -2.2170120
O       -0.1310460       0.2835230      -2.1916250
64
MnBnTPEN_Peroxide_Mn4_G3.log
64
Final Energy =        -2620.2192983700
C       -3.2194060      -0.0934440       0.9985960
C       -3.5377400       0.6221170      -1.2009100
C       -4.9056180       0.7581240      -0.9930290
C       -5.4371830       0.4420210       0.2584050
C       -4.5781220       0.0194490       1.2738360
H       -3.0711900       0.8612390      -2.1554240
H       -5.5377790       1.1123670      -1.8075560
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H	-6.5074260	0.5395930	0.4484860
H	-4.9483060	-0.2095150	2.2734130
C	-2.1847810	-0.5076990	1.9952430
H	-2.0393670	-1.5964580	1.9701030
H	-2.4664940	-0.2409130	3.0246620
N	-0.9106090	0.1512210	1.6034270
C	0.2438940	-0.4958590	2.2788730
H	0.2727530	-0.2195440	3.3438100
H	0.1084130	-1.5825890	2.2281250
C	1.4924900	-0.0598510	1.5671180
H	1.6419630	1.0195570	1.6928930
H	2.3808670	-0.5579790	1.9792950
N	1.3658060	-0.3328150	0.1062020
C	-0.9835030	1.6214300	1.9108770
H	-0.3828560	1.8478020	2.8027020
H	-2.0221120	1.8685550	2.1742720
C	-0.5887080	2.4981110	0.7558550
C	-0.3655430	3.8665380	0.9101200
C	-0.1101330	4.6373690	-0.2230110
H	-0.4006250	4.3140880	1.9040740
C	-0.3007350	2.6533120	-1.5576740
C	-0.0890110	4.0233700	-1.4791280
H	0.0682340	5.7099370	-0.1278880
H	-0.2734610	2.1116150	-2.5030730
H	0.1000080	4.5945150	-2.3882900
C	1.6446820	-1.7628600	-0.2109660
H	2.4806660	-2.1406060	0.3935370
H	1.9558780	-1.8068400	-1.2635460
C	2.3251160	0.5601050	-0.6484980
H	2.0348000	1.5914480	-0.4205760
H	2.1509980	0.3884900	-1.7147950
C	0.4424340	-2.6551600	-0.0976220
C	0.5591480	-4.0317170	0.0901000
C	-1.8581740	-2.8428750	-0.4390430
C	-0.5849120	-4.8249870	0.0052250
H	1.5384020	-4.4696540	0.2860970
C	-1.8125760	-4.2226350	-0.2804010
H	-2.7933350	-2.3284450	-0.6580260
H	-0.5172450	-5.9046190	0.1502800
H	-2.7274010	-4.8077410	-0.3758740
C	3.7816260	0.3441270	-0.3074860
C	4.5512130	-0.5906300	-1.0182610
C	4.3954550	1.0823560	0.7169660
C	5.8929690	-0.8039780	-0.6941670
H	4.1036830	-1.1498330	-1.8429460
C	5.7373960	0.8719870	1.0423970
H	3.8247660	1.8397990	1.2592320
C	6.4875080	-0.0771690	0.3416290
H	6.4773140	-1.5344500	-1.2579890
H	6.1996700	1.4561840	1.8411200
H	7.5373780	-0.2417620	0.5944480
N	-2.7196070	0.1847860	-0.2267150
N	-0.5331620	1.9173220	-0.4558320
N	-0.7569340	-2.0806530	-0.3211330

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Mn       -0.6912210      -0.0749550      -0.4604210
O         0.1024190      -0.2258810      -2.1074300
O        -1.2290250      -0.2314580      -2.2990660
65
OSS_MnBnTPEN_Hydroperoxo_G1.log
65
Final Energy =        -2620.8531867700
C        -3.2632030       0.0702690      -0.8717220
C        -3.4275630      -0.3704120       1.4201570
C        -4.8118280      -0.4844450       1.3359330
C        -5.4272160      -0.3152400       0.0937470
C        -4.6418390      -0.0389210      -1.0281030
H        -2.8856480      -0.4895770       2.3598220
H        -5.3917050      -0.7064720       2.2321650
H        -6.5105890      -0.4048730      -0.0040410
H        -5.0874280       0.0878260      -2.0153110
C        -2.3076930       0.4030690      -1.9887940
H        -2.1478740       1.4900010      -2.0292890
H        -2.7051090       0.0991980      -2.9684870
N        -1.0098240      -0.2567280      -1.6966850
C         0.1535930       0.3579580      -2.3840540
H         0.2002340       0.0466550      -3.4394400
H         0.0289810       1.4473570      -2.3732720
C         1.4124570      -0.0649310      -1.6529960
H         1.5308530      -1.1541040      -1.7190280
H         2.3012070       0.3827280      -2.1207690
N         1.3443100       0.2927650      -0.2019440
C        -1.1099870      -1.7234100      -1.9722780
H        -0.4839300      -1.9863690      -2.8376520
H        -2.1424410      -1.9592530      -2.2680310
C        -0.7594620      -2.5804410      -0.7882540
C        -0.6630410      -3.9690270      -0.8972460
C        -0.4022770      -4.7197620       0.2465100
H        -0.7972540      -4.4456370      -1.8693500
C        -0.3448450      -2.6768760       1.5020660
C        -0.2480590      -4.0613980       1.4701980
H        -0.3222860      -5.8066160       0.1857590
H        -0.2188990      -2.1038460       2.4209560
H        -0.0487340      -4.6102630       2.3909740
C         1.6891280       1.7230360       0.0195360
H         2.5139030       2.0390210      -0.6342970
H         2.0333440       1.8193040       1.0580830
C         2.2614470      -0.5842680       0.6109990
H         1.9543660      -1.6193720       0.4269630
H         2.0538710      -0.3476000       1.6609550
C         0.5059090       2.6331490      -0.1026760
C         0.6429930       4.0002360      -0.3408670
C        -1.7850160       2.8680100       0.2443580
C        -0.4860830       4.8148530      -0.2756830
H         1.6276840       4.4133050      -0.5620570
C        -1.7204780       4.2400040       0.0382120
H        -2.7293300       2.3817100       0.4857170
H        -0.4033250       5.8876610      -0.4588900
H        -2.6265930       4.8408720       0.1177740
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C       3.7320770      -0.4172860       0.3080480
C       4.3422290      -1.1548590      -0.7191740
C       4.5164680       0.4788180       1.0510770
C       5.6963440      -0.9810600      -1.0146660
H       3.7589590      -1.8839220      -1.2861250
C       5.8710960       0.6543870       0.7584130
H       4.0677900       1.0378510       1.8757390
C       6.4626790      -0.0710500      -0.2799880
H       6.1557910      -1.5639090      -1.8160870
H       6.4671540       1.3548500       1.3476090
H       7.5222110       0.0640130      -0.5090270
N      -2.6824260      -0.0951580       0.3385770
N      -0.5876950      -1.9560420       0.3898840
N      -0.6974160       2.0793640       0.1517960
Mn     -0.6656950       0.0698190       0.3552600
O      -0.4677680       0.1093590       2.1232120
O       0.2807280       1.2003500       2.6717790
H       0.5278670       0.8344900       3.5392920
65
OSS_MnBnTPEN_Hydroperoxo_G2.log
65
Final Energy =            -2620.8531867700
C       3.2631880       0.0705240       0.8716320
C       3.4276000      -0.3704420      -1.4201990
C       4.8117630      -0.4855260      -1.3357280
C       5.4270690      -0.3166990      -0.0934560
C       4.6417090      -0.0396910       1.0282420
H       2.8857330      -0.4892600      -2.3599360
H       5.3916250      -0.7080830      -2.2318380
H       6.5103530      -0.4071900       0.0045280
H       5.0872330       0.0868000       2.0155130
C       2.3076320       0.4037750       1.9885230
H       2.1476710       1.4906970       2.0285280
H       2.7049650       0.1003400       2.9683790
N       1.0098140      -0.2562520       1.6965200
C      -0.1536220       0.3582990       2.3839730
H      -0.2001610       0.0469700       3.4393510
H      -0.0291360       1.4477130       2.3732130
C      -1.4124680      -0.0647390       1.6529530
H      -1.5307620      -1.1539200       1.7190680
H      -2.3012900       0.3828820       2.1206230
N      -1.3442810       0.2928170       0.2018780
C       1.1102700      -1.7229030       1.9722590
H       0.4844670      -1.9858670       2.8378080
H       2.1428330      -1.9585630       2.2677940
C       0.7595900      -2.5801090       0.7883980
C       0.6629510      -3.9686580       0.8976610
C       0.4020190      -4.7195870      -0.2459310
H       0.7971340      -4.4450840       1.8698600
C       0.3448520      -2.6769290      -1.5018740
C       0.2478510      -4.0614290      -1.4697380
H       0.3218560      -5.8064160      -0.1849640
H       0.2189200      -2.1040770      -2.4208780
H       0.0483740      -4.6104220      -2.3904050
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C        -1.6891630         1.7230460        -0.0198420
H        -2.5142170         2.0390210         0.6336380
H        -2.0329780         1.8191310        -1.0585510
C        -2.2613030        -0.5843180        -0.6110280
H        -1.9541420        -1.6193910        -0.4269440
H        -2.0537420        -0.3477080        -1.6610100
C        -0.5060400         2.6332350         0.1026710
C        -0.6431430         4.0002200         0.3414070
C         1.7847900         2.8683130        -0.2448200
C         0.4858930         4.8149090         0.2762670
H        -1.6278000         4.4131650         0.5629690
C         1.7202310         4.2402390        -0.0381790
H         2.7290480         2.3821200        -0.4866180
H         0.4031350         5.8876430         0.4599050
H         2.6262870         4.8411900        -0.1177840
C        -3.7319480        -0.4175000        -0.3080590
C        -4.3419970        -1.1552140         0.7191220
C        -4.5164460         0.4785840        -1.0509970
C        -5.6961350        -0.9816200         1.0146240
H        -3.7586220        -1.8842290         1.2860340
C        -5.8711000         0.6539460        -0.7583260
H        -4.0678450         1.0377580        -1.8756030
C        -6.4625920        -0.0716600         0.2800080
H        -6.1555050        -1.5645850         1.8160050
H        -6.4672450         1.3543820        -1.3474650
H        -7.5221430         0.0632400         0.5090530
N         2.6824830        -0.0945090        -0.3387780
N         0.5878620        -1.9558980        -0.3898570
N         0.6972580         2.0795940        -0.1522180
Mn        0.6656980         0.0699870        -0.3554920
O         0.4675970         0.1091320        -2.1233740
O        -0.2800380         1.2007000        -2.6720910
H        -0.5276510         0.8347690        -3.5394390
65
OSS_MnBnTPEN_Hydroperoxo_G3.log
65
Final Energy =          -2620.8432176000
C        -2.9531710        -1.3648620         0.4517600
C        -2.6265380        -1.0953310        -1.8481300
C        -3.7942770        -1.7969650        -2.1313340
C        -4.5526340        -2.3016820        -1.0733250
C        -4.1304610        -2.0750240         0.2386070
H        -1.9881980        -0.6931640        -2.6334300
H        -4.0987630        -1.9401600        -3.1683640
H        -5.4726920        -2.8563960        -1.2658600
H        -4.7092740        -2.4330620         1.0905970
C        -2.3936130        -1.0351410         1.8099970
H        -1.6843720        -1.8141510         2.1255140
H        -3.1855750        -0.9760180         2.5721030
N        -1.6563690         0.2455880         1.6773630
C        -0.7222410         0.5284000         2.7956500
H        -1.2467690         1.0119930         3.6333830
H        -0.3377350        -0.4287980         3.1697550
C         0.4034440         1.4071630         2.2855250
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H      0.0184420      2.3675260      1.9211170
H      1.1181720      1.6320960      3.0932720
N      1.1041310      0.7217760      1.1572790
C     -2.6178840      1.3692250      1.4809420
H     -2.8233940      1.8662200      2.4399640
H     -3.5760780      0.9552440      1.1338230
C     -2.1497300      2.3484630      0.4464640
C     -2.6808270      3.6335860      0.3430080
C     -2.2734340      4.4491010     -0.7116770
H     -3.4079680      3.9798000      1.0786310
C     -0.8583600      2.6641570     -1.4633020
C     -1.3517990      3.9517370     -1.6360120
H     -2.6733740      5.4596250     -0.8129190
H     -0.1396690      2.2221280     -2.1538120
H     -1.0115510      4.5511220     -2.4807950
C      1.8759800     -0.4360260      1.6996070
H      1.6788670     -0.5410140      2.7761190
H      2.9530550     -0.2528480      1.6164150
C      1.9964960      1.7322760      0.4497990
H      2.2526170      2.5079660      1.1853610
H      1.3886820      2.2122840     -0.3247910
C      1.5283390     -1.7291180      1.0301970
C      2.3398940     -2.8551680      1.1813400
C     -0.0026070     -2.9416860     -0.2318270
C      1.9398520     -4.0615100      0.6147790
H      3.2717310     -2.7733160      1.7421540
C      0.7396520     -4.1057570     -0.0999950
H     -0.9223370     -2.9345570     -0.8110500
H      2.5568110     -4.9553070      0.7240230
H      0.3857940     -5.0256360     -0.5659350
C      3.2819590      1.1932740     -0.1294360
C      3.3083030      0.2504180     -1.1701960
C      4.5003480      1.6507660      0.3970910
C      4.5261010     -0.2253730     -1.6609080
H      2.3801570     -0.1251750     -1.5929040
C      5.7191580      1.1831670     -0.1025100
H      4.4940970      2.3798590      1.2112340
C      5.7347470      0.2394230     -1.1324430
H      4.5286780     -0.9642530     -2.4656920
H      6.6562760      1.5540900      0.3186500
H      6.6848010     -0.1337360     -1.5217920
N     -2.2170330     -0.8999730     -0.5837290
N     -1.2414870      1.8861760     -0.4333380
N      0.3769370     -1.7751500      0.3295190
Mn    -0.4921490      0.0235460     -0.0689360
O      0.1927070      0.0864890     -1.7173070
O      0.4731060     -1.1311210     -2.4110070
H      0.6033500     -0.7979550     -3.3165300
63
OSS_MnBnTPEN_Oxo_G1.log
63
Final Energy =        -2544.8819056900
C      3.0150020      0.4298970     -0.3424300
C      2.0569400     -0.3976030     -2.3238000
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C      3.2988830     -0.4396080     -2.9448280
C      4.4282550     -0.0388740     -2.2288550
C      4.2833740      0.3979090     -0.9105470
H      1.1471320     -0.6959090     -2.8442240
H      3.3684100     -0.7863200     -3.9759460
H      5.4164380     -0.0695730     -2.6906410
H      5.1431990      0.7114760     -0.3183320
C      2.7309470      0.9336200      1.0444210
H      2.4927600      2.0059690      1.0105930
H      3.6048140      0.8241950      1.7019980
N      1.5563040      0.1949450      1.5647500
C      0.8134770      0.9025290      2.6389460
H      1.3325250      0.8125160      3.6052890
H      0.7668210      1.9712760      2.4008840
C     -0.5583890      0.2727140      2.7153150
H     -0.4848020     -0.7891580      2.9833360
H     -1.1783930      0.7577130      3.4817960
N     -1.2545160      0.3542100      1.3844630
C      1.9666180     -1.1657390      2.0243410
H      1.8087700     -1.2642420      3.1074920
H      3.0485110     -1.2878430      1.8702410
C      1.2760890     -2.2619000      1.2790570
C      1.4990480     -3.6045940      1.5890140
C      0.9621190     -4.5911180      0.7685590
H      2.1104580     -3.8585880      2.4556370
C      0.0331610     -2.8590340     -0.6019750
C      0.2376030     -4.2077190     -0.3643060
H      1.1266160     -5.6461510      0.9933200
H     -0.5098700     -2.5172360     -1.4800230
H     -0.1690860     -4.9405780     -1.0612530
C     -1.7902780      1.7292320      1.1669220
H     -2.2135520      2.1281470      2.0992450
H     -2.6076330      1.6651600      0.4374100
C     -2.3914080     -0.6619720      1.4014010
H     -2.9781690     -0.4393050      2.3064760
H     -1.9243360     -1.6432470      1.5364090
C     -0.7867450      2.6501870      0.5619210
C     -0.8896590      4.0351490      0.6559020
C      0.9697460      2.8286720     -0.9720470
C     -0.0262660      4.8284270     -0.0970080
H     -1.6499710      4.4751720      1.3012470
C      0.9034250      4.2128600     -0.9400310
H      1.6831390      2.3210590     -1.6158290
H     -0.0865200      5.9163290     -0.0374710
H      1.5795310      4.7932240     -1.5675150
C     -3.2932480     -0.6526830      0.2035050
C     -4.3685350      0.2455280      0.0976580
C     -3.0981600     -1.5979310     -0.8367170
C     -5.1638050      0.2558870     -1.0456260
H     -4.5962060      0.9319220      0.9149150
C     -3.8914000     -1.5826620     -1.9883040
H     -2.3662300     -2.3896900     -0.7006120
C     -4.9143760     -0.6477750     -2.1014960
H     -5.9918990      0.9627340     -1.1221800
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H      -3.7181560      -2.3177220      -2.7755910
H      -5.5475800      -0.6282010      -2.9904210
N       1.9303840       0.0307170      -1.0521000
N       0.5069340      -1.9059830       0.2336910
N       0.1566500       2.0651400      -0.2092550
Mn      0.1611240       0.0628850      -0.1206710
O      -0.8399530      -0.2286060      -1.2692870
63
OSS_MnBnTPEN_Oxo_G2.log
63
Final Energy =        -2544.8819053700
C       3.0148680       0.4304000      -0.3423740
C       2.0569710      -0.3972770      -2.3237350
C       3.2989410      -0.4392000      -2.9447240
C       4.4282450      -0.0382930      -2.2287340
C       4.2832710       0.3985480      -0.9104510
H       1.1472070      -0.6957060      -2.8441760
H       3.3685360      -0.7859720      -3.9758170
H       5.4164450      -0.0688940      -2.6904910
H       5.1430460       0.7122640      -0.3182420
C       2.7307530       0.9342430       1.0444100
H       2.4924190       2.0065580       1.0104390
H       3.6046620       0.8250340       1.7019700
N       1.5562100       0.1954940       1.5648460
C       0.8131800       0.9032040       2.6388250
H       1.3322160       0.8135880       3.6052090
H       0.7662740       1.9718650       2.4004470
C      -0.5585510       0.2730880       2.7153560
H      -0.4847170      -0.7887020       2.9836230
H      -1.1786910       0.7581090       3.4817130
N      -1.2546880       0.3540920       1.3844930
C       1.9666180      -1.1650790       2.0247420
H       1.8084070      -1.2634940       3.1078420
H       3.0485910      -1.2870180       1.8710500
C       1.2765490      -2.2614700       1.2793430
C       1.4998280      -3.6041090       1.5892870
C       0.9634240      -4.5907520       0.7686330
H       2.1111090      -3.8579500       2.4560490
C       0.0343180      -2.8588660      -0.6020660
C       0.2391310      -4.2075060      -0.3644280
H       1.1281850      -5.6457440       0.9933940
H      -0.5085980      -2.5172280      -1.4802470
H      -0.1671000      -4.9404380      -1.0615640
C      -1.7909350       1.7288840       1.1667480
H      -2.2143010       2.1277990       2.0990330
H      -2.6083090       1.6644230       0.4372920
C      -2.3912210      -0.6624440       1.4016000
H      -2.9780950      -0.4398010       2.3066090
H      -1.9238370      -1.6435500       1.5367810
C      -0.7877150       2.6501100       0.5616220
C      -0.8912340       4.0350480       0.6552740
C       0.9690430       2.8290000      -0.9719920
C      -0.0280090       4.8285260      -0.0976130
H      -1.6518880       4.4749000       1.3003340
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C       0.9021560       4.2131670      -0.9402590
H       1.6827790       2.3215720      -1.6155320
H      -0.0887470       5.9164160      -0.0383360
H       1.5781820       4.7936820      -1.5676890
C      -3.2930010      -0.6536300       0.2036320
C      -3.0973040      -1.5987940      -0.8365680
C      -4.3686330       0.2440900       0.0976050
C      -3.8903650      -1.5838800      -1.9883180
H      -2.3651250      -2.3902890      -0.7002690
C      -5.1637170       0.2540930      -1.0458300
H      -4.5966920       0.9304140       0.9148140
C      -4.9137150      -0.6494580      -2.1016720
H      -3.7166410      -2.3188750      -2.7755620
H      -5.9920950       0.9605890      -1.1225520
H      -5.5467940      -0.6301050      -2.9906880
N       1.9303430       0.0310740      -1.0520750
N       0.5075400      -1.9057280       0.2338210
N       0.1560770       2.0652760      -0.2092350
Mn      0.1610730       0.0630220      -0.1205680
O      -0.8398770      -0.2287890      -1.2692570
63
OSS_MnBnTPEN_Oxo_G3.log
63
Final Energy =       -2544.8827567900
C       3.2153230       0.0519260       0.7907190
C       3.3560140      -0.6049140      -1.4666900
C       4.7314860      -0.7640840      -1.3633480
C       5.3582110      -0.5000700      -0.1443700
C       4.5880680      -0.0947290       0.9476000
H       2.8299370      -0.7973770      -2.4006480
H       5.2943080      -1.0920120      -2.2374590
H       6.4376290      -0.6200580      -0.0394800
H       5.0381140       0.0994700       1.9214310
C       2.2773900       0.4811500       1.8788160
H       2.1679540       1.5738480       1.8879510
H       2.6481640       0.1909240       2.8718370
N       0.9647480      -0.1445170       1.5847300
C      -0.1812950       0.5383390       2.2372960
H      -0.2465350       0.2702160       3.3023620
H      -0.0270580       1.6221330       2.1872310
C      -1.4287200       0.1097910       1.5064980
H      -1.5928840      -0.9676230       1.6225150
H      -2.3174750       0.6203540       1.8977780
N      -1.2990530       0.3863210       0.0347520
C       1.0169600      -1.5947060       1.9439930
H       0.4322420      -1.7819650       2.8557600
H       2.0533700      -1.8653490       2.1923340
C       0.5723450      -2.4820870       0.8262160
C       0.3603250      -3.8478280       1.0136710
C       0.0487000      -4.6449990      -0.0839580
H       0.4522260      -4.2708280       2.0144590
C       0.1594570      -2.6911860      -1.4700460
C      -0.0418670      -4.0558380      -1.3485900
H      -0.1181800      -5.7157950       0.0429890
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H        0.0792540      -2.1910400      -2.4344680
H       -0.2757360      -4.6406670      -2.2382470
C       -1.5594980       1.8255030      -0.2767930
H       -2.3972940       2.1996310       0.3246430
H       -1.8576980       1.8923680      -1.3333420
C       -2.2669000      -0.4992320      -0.7544740
H       -1.9963410      -1.5330810      -0.5262780
H       -2.0654710      -0.3076870      -1.8153810
C       -0.3377270       2.6683080      -0.1169850
C       -0.3932800       4.0424020       0.0891580
C        1.9881010       2.7506490      -0.4026280
C        0.7889300       4.7807910       0.0420410
H       -1.3562720       4.5204610       0.2692750
C        1.9936480       4.1259410      -0.2284770
H        2.9081440       2.2106280      -0.6123650
H        0.7688550       5.8598180       0.2031110
H        2.9365570       4.6676260      -0.3007640
C       -3.7121030      -0.2532170      -0.4178730
C       -4.3424410      -1.0022340       0.5908460
C       -4.4580800       0.7085380      -1.1210340
C       -5.6823200      -0.7775700       0.9064770
H       -3.7882560      -1.7786210       1.1226260
C       -5.7985690       0.9320200      -0.8063970
H       -3.9973100       1.2729960      -1.9343130
C       -6.4107360       0.1951450       0.2131030
H       -6.1618130      -1.3685120       1.6893180
H       -6.3693790       1.6771010      -1.3640650
H       -7.4601210       0.3707260       0.4594530
N        2.6274050      -0.1918760      -0.4075600
N        0.4504340      -1.9227790      -0.3928320
N        0.8434810       2.0385280      -0.3194970
Mn       0.6607220       0.0730190      -0.5774050
O        0.4131730       0.0637800      -2.0748660
64
OSS_MnBnTPEN_Peroxide_Mn3_G1.log
64
Final Energy =          -2620.3804956900
C        3.3291550      -0.0053270       0.8788960
C        3.6136230      -0.4242400      -1.3856390
C        4.9895970      -0.5724820      -1.2253670
C        5.5425730      -0.4331800       0.0480660
C        4.6942180      -0.1453970       1.1187630
H        3.1290500      -0.4995020      -2.3589790
H        5.6117800      -0.7946260      -2.0933950
H        6.6162280      -0.5493180       0.2078640
H        5.0793580      -0.0300030       2.1327450
C        2.3364920       0.3537430       1.9445270
H        2.2026850       1.4450220       1.9619820
H        2.6859410       0.0552440       2.9463280
N        1.0407370      -0.2660810       1.6041290
C       -0.0746270       0.4032720       2.3112870
H       -0.0886160       0.1235360       3.3783330
H        0.0932230       1.4863880       2.2639760
C       -1.3820650       0.0314960       1.6519530
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H        -1.5694510       -1.0420170        1.7855120
H        -2.2178800        0.5643390        2.1330440
N        -1.3332950        0.3033610        0.1963170
C         1.0890900       -1.7262860        1.8919990
H         0.6478910       -1.9425860        2.8774050
H         2.1455960       -2.0279340        1.9564220
C         0.4597430       -2.5663540        0.8151890
C         0.0492930       -3.8807790        1.0435560
C        -0.4177880       -4.6376440       -0.0317130
H         0.1046920       -4.3005840        2.0491190
C        -0.0459750       -2.7335560       -1.4463110
C        -0.4551340       -4.0557120       -1.3013390
H        -0.7460300       -5.6678300        0.1198890
H        -0.0525610       -2.2062570       -2.4006710
H        -0.8081960       -4.6127490       -2.1702720
C        -1.5680360        1.7310710       -0.1181510
H        -2.3910560        2.1446600        0.4850370
H        -1.8820890        1.7796750       -1.1700470
C        -2.3260370       -0.5500310       -0.5321040
H        -2.1399510       -1.5849000       -0.2242930
H        -2.0674990       -0.4622320       -1.5940390
C        -0.3452420        2.6010870       -0.0134890
C        -0.4498030        3.9665060        0.2580840
C         1.9373930        2.7946250       -0.3781060
C         0.6930510        4.7636890        0.1940120
H        -1.4221840        4.3941940        0.5069760
C         1.9084460        4.1669220       -0.1459650
H         2.8693850        2.2916780       -0.6352830
H         0.6342260        5.8339940        0.4007880
H         2.8276730        4.7485980       -0.2252110
C        -3.7769650       -0.2015720       -0.2869520
C        -4.4683050       -0.7178920        0.8211790
C        -4.4646970        0.6491370       -1.1666920
C        -5.8019120       -0.3743610        1.0573860
H        -3.9640980       -1.4081940        1.5011460
C        -5.7985270        0.9950720       -0.9349050
H        -3.9524850        1.0393280       -2.0497650
C        -6.4693840        0.4881480        0.1821510
H        -6.3235560       -0.7874650        1.9239180
H        -6.3167940        1.6576820       -1.6320320
H        -7.5127430        0.7559570        0.3646230
N         2.7975390       -0.1502700       -0.3539290
N         0.3923490       -2.0052120       -0.4050140
N         0.8398750        2.0237720       -0.2976730
Mn        0.7254120       -0.0086530       -0.5168200
O         1.0654540       -0.3018760       -2.3524380
O        -0.1001220        0.4210650       -2.1762250
64
OSS_MnBnTPEN_Peroxide_Mn3_G2.log
64
Final Energy =          -2620.3804957400
C         3.3291610       -0.0055120        0.8786200
C         3.6136420       -0.4245380       -1.3858760
C         4.9896570       -0.5722520       -1.2256890
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C	5.5426980	-0.4326050	0.0476970
C	4.6943120	-0.1450410	1.1184100
H	3.1289710	-0.5000360	-2.3591550
H	5.6118580	-0.7942290	-2.0937480
H	6.6164130	-0.5483160	0.2073910
H	5.0794380	-0.0293790	2.1323670
C	2.3365760	0.3533640	1.9444140
H	2.2027780	1.4446420	1.9621060
H	2.6861930	0.0546920	2.9461040
N	1.0407930	-0.2664280	1.6041160
C	-0.0745630	0.4028390	2.3113750
H	-0.0886430	0.1228490	3.3783530
H	0.0933550	1.4859540	2.2643100
C	-1.3820240	0.0312830	1.6519430
H	-1.5695040	-1.0422300	1.7853500
H	-2.2177580	0.5641440	2.1331620
N	-1.3332830	0.3033780	0.1963510
C	1.0892290	-1.7266500	1.8919230
H	0.6484450	-1.9429570	2.8775140
H	2.1457660	-2.0282900	1.9558710
C	0.4594430	-2.5666350	0.8153210
C	0.0486910	-3.8809520	1.0437780
C	-0.4187980	-4.6376880	-0.0314010
H	0.1041600	-4.3007700	2.0493300
C	-0.0467410	-2.7337320	-1.4460930
C	-0.4562330	-4.0557810	-1.3010320
H	-0.7472770	-5.6677890	0.1202810
H	-0.0532810	-2.2064070	-2.4004440
H	-0.8096030	-4.6127530	-2.1698800
C	-1.5677390	1.7311650	-0.1178580
H	-2.3906520	2.1448270	0.4854370
H	-1.8818620	1.7800210	-1.1697190
C	-2.3261460	-0.5496520	-0.5322680
H	-2.1402730	-1.5846420	-0.2247410
H	-2.0675760	-0.4615920	-1.5941830
C	-0.3447810	2.6009590	-0.0131790
C	-0.4491470	3.9663840	0.2584450
C	1.9378620	2.7942280	-0.3779020
C	0.6937980	4.7634320	0.1943050
H	-1.4214520	4.3941950	0.5074250
C	1.9090970	4.1665310	-0.1457660
H	2.8697930	2.2911760	-0.6350990
H	0.6351200	5.8337400	0.4011080
H	2.8283730	4.7481170	-0.2250990
C	-3.7770310	-0.2010020	-0.2871070
C	-4.4684650	-0.7171970	0.8210280
C	-4.4646150	0.6498060	-1.1668630
C	-5.8020040	-0.3734050	1.0572320
H	-3.9644170	-1.4076190	1.5009880
C	-5.7983800	0.9959950	-0.9350790
H	-3.9523050	1.0398720	-2.0499370
C	-6.4693180	0.4892240	0.1819930
H	-6.3237230	-0.7864020	1.9237700
H	-6.3165420	1.6586800	-1.6322140

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H     -7.5126230      0.7572400      0.3644690
N      2.7974990     -0.1507790     -0.3541310
N      0.3919650     -2.0055210     -0.4048720
N      0.8402620      2.0235070     -0.2974150
Mn     0.7254100     -0.0089230     -0.5168790
O      1.0650840     -0.3024650     -2.3524740
O     -0.0998520      0.4214470     -2.1762400
64
OSS_MnBnTPEN_Peroxide_Mn3_G3.log
64
Final Energy =        -2620.3714901600
C      2.2980010      2.0606730      0.8600970
C      2.2335990      2.2433690     -1.4511760
C      2.9989020      3.4073210     -1.4200300
C      3.4156440      3.9113010     -0.1882060
C      3.0644230      3.2177370      0.9715230
H      1.8662530      1.8171960     -2.3847300
H      3.2594230      3.9039080     -2.3555700
H      4.0155360      4.8214180     -0.1292010
H      3.3858080      3.5593220      1.9564760
C      1.8879350      1.2255840      2.0369570
H      0.9119650      1.5694580      2.4103530
H      2.6110390      1.3180890      2.8648380
N      1.7449150     -0.1662940      1.5711030
C      1.0938220     -1.0499430      2.5771460
H      1.8396740     -1.6922540      3.0673760
H      0.6690900     -0.4248010      3.3716840
C      0.0259570     -1.9143680      1.9301530
H      0.4806640     -2.7216300      1.3430610
H     -0.5924520     -2.3872560      2.7140540
N     -0.8103000     -1.1114940      1.0121970
C      3.0657660     -0.7224000      1.1852120
H      3.6265300     -1.0556220      2.0720400
H      3.6598520      0.0706180      0.7090430
C      2.8832730     -1.8257320      0.1887470
C      3.7545560     -2.9064870      0.0601710
C      3.5266000     -3.8319480     -0.9599820
H      4.5955450     -3.0125270      0.7470200
C      1.6074470     -2.5396930     -1.6125320
C      2.4366430     -3.6413530     -1.8120560
H      4.1900920     -4.6899140     -1.0859590
H      0.7292480     -2.3336140     -2.2258370
H      2.2222380     -4.3399680     -2.6221150
C     -1.5403730     -0.0607430      1.7639850
H     -0.9092220      0.2884560      2.5896890
H     -2.4573030     -0.4489940      2.2268140
C     -1.7490360     -2.0507450      0.2770430
H     -1.8960880     -2.9304750      0.9220700
H     -1.2253960     -2.3691560     -0.6310000
C     -1.8291190      1.1114530      0.8786170
C     -2.9778550      1.8932380      0.9937900
C     -1.0617750      2.3750710     -0.9035610
C     -3.1542620      2.9624230      0.1176330
H     -3.7301480      1.6411380      1.7418990
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C       -2.1816600       3.2003960      -0.8565480
H       -0.2957450       2.4973700      -1.6680350
H       -4.0471230       3.5876760       0.1789230
H       -2.2884560       4.0090020      -1.5809370
C       -3.1127700      -1.4911250      -0.0601090
C       -3.3399940      -0.7235410      -1.2131820
C       -4.1906850      -1.7361740       0.8069130
C       -4.6067680      -0.1980250      -1.4769690
H       -2.5001090      -0.5168040      -1.8767830
C       -5.4567800      -1.2051130       0.5482960
H       -4.0363650      -2.3488610       1.6992760
C       -5.6668920      -0.4286650      -0.5955110
H       -4.7640660       0.4053110      -2.3743630
H       -6.2804710      -1.4020000       1.2385420
H       -6.6553120      -0.0104470      -0.8008020
N        1.8804400       1.5866140      -0.3334130
N        1.8264210      -1.6566260      -0.6243330
N       -0.8776450       1.3666390      -0.0376110
Mn       0.5949980      -0.0430760      -0.2946860
O       -0.4511760      -0.5741830      -1.7841520
O        0.6819200       0.1298480      -2.1839480
65
Quitnet_MnBnTPEN_Hydroperoxo_G1.log
65
Final Energy =            -2620.8816465200
C       -3.4097700      -0.0823610      -0.9868020
C       -3.8508950      -0.4614210       1.2708400
C       -5.2102500      -0.6307010       1.0203140
C       -5.6650620      -0.5191780      -0.2957630
C       -4.7530970      -0.2446210      -1.3182510
H       -3.4328420      -0.5342330       2.2779160
H       -5.8941670      -0.8478570       1.8413320
H       -6.7235840      -0.6512050      -0.5277630
H       -5.0767900      -0.1604910      -2.3564100
C       -2.3398850       0.2685450      -1.9900320
H       -2.2192050       1.3607330      -2.0278100
H       -2.6139650      -0.0593030      -3.0042890
N       -1.0418410      -0.3281710      -1.5772290
C        0.1007420       0.3231050      -2.2765190
H        0.1307980      -0.0006690      -3.3288950
H       -0.0791330       1.4048630      -2.2785490
C        1.4161360      -0.0080250      -1.5964260
H        1.6018500      -1.0883750      -1.6581380
H        2.2381540       0.4836730      -2.1415730
N        1.4146460       0.3691380      -0.1648510
C       -1.0760130      -1.8055750      -1.8163000
H       -0.6150960      -2.0414300      -2.7866260
H       -2.1296040      -2.1145890      -1.8907140
C       -0.4633480      -2.6151470      -0.7087970
C       -0.0400630      -3.9305780      -0.8963140
C        0.3932490      -4.6632480       0.2089240
H       -0.0609350      -4.3712800      -1.8935770
C       -0.0232230      -2.7450500       1.5842470
C        0.3903050      -4.0664720       1.4730140
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H        0.7281170      -5.6947130       0.0848720
H       -0.0337230      -2.2128330       2.5364500
H        0.7133160      -4.6108600       2.3605650
C        1.6331700       1.8102240       0.0504050
H        2.4140880       2.2076930      -0.6166340
H        1.9972170       1.9397590       1.0800510
C        2.3978550      -0.4401230       0.6163950
H        2.1407890      -1.4952450       0.4668430
H        2.2298360      -0.2011590       1.6737040
C        0.3891800       2.6559270      -0.0476470
C        0.4696440       4.0197730      -0.3365870
C       -1.9081760       2.8311220       0.3258890
C       -0.6847380       4.7979690      -0.2795200
H        1.4338430       4.4592990      -0.5950790
C       -1.8966640       4.1955360       0.0699630
H       -2.8297420       2.3124750       0.5922040
H       -0.6399520       5.8656880      -0.5020170
H       -2.8219830       4.7679710       0.1372210
C        3.8476760      -0.2113790       0.2510090
C        4.4506420      -0.9494140      -0.7799300
C        4.6128860       0.7527490       0.9252260
C        5.7786630      -0.7135730      -1.1438890
H        3.8820690      -1.7264500      -1.2963610
C        5.9414600       0.9906700       0.5641320
H        4.1705020       1.3172020       1.7496390
C        6.5258650       0.2613080      -0.4756360
H        6.2332120      -1.2980810      -1.9470100
H        6.5233140       1.7433130       1.1010090
H        7.5651360       0.4448530      -0.7577910
N       -2.9832250      -0.1924170       0.2853530
N       -0.4295460      -2.0428240       0.5111400
N       -0.7913090       2.0823970       0.2527930
Mn      -0.8008210      -0.0031630       0.5310020
O       -0.8119760       0.0798320       2.3556550
O        0.2040190       0.9645100       2.8185600
H        0.7138340       0.3883610       3.4165320
65
Quitnet_MnBnTPEN_Hydroperoxo_G2.log
65
Final Energy =            -2620.8816464100
C        3.4097840      -0.0822000       0.9867530
C        3.8508320      -0.4611340      -1.2709290
C        5.2101780      -0.6305570      -1.0204380
C        5.6650230      -0.5191820       0.2956380
C        4.7530990      -0.2446220       1.3181650
H        3.4327510      -0.5338500      -2.2780000
H        5.8940610      -0.8477100      -1.8414840
H        6.7235340      -0.6513320       0.5276140
H        5.0768160      -0.1606190       2.3563260
C        2.3399490       0.2687230       1.9900160
H        2.2192290       1.3609100       2.0277110
H        2.6141080      -0.0590240       3.0042850
N        1.0419010      -0.3280620       1.5773280
C       -0.1006700       0.3232080       2.2766270
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H      -0.1306860     -0.0005000      3.3290260
H       0.0791460      1.4049740      2.2785870
C      -1.4160630     -0.0080550      1.5965860
H      -1.6016050     -1.0884360      1.6582830
H      -2.2381200      0.4835220      2.1417810
N      -1.4146850      0.3691180      0.1650220
C       1.0760640     -1.8054520      1.8163840
H       0.6149060     -2.0413630      2.7865780
H       2.1296390     -2.1144560      1.8910560
C       0.4636360     -2.6150670      0.7087740
C       0.0404490     -3.9305440      0.8963170
C      -0.3927260     -4.6632750     -0.2089240
H       0.0612950     -4.3711550      1.8936210
C       0.0236760     -2.7450730     -1.5842810
C      -0.3897440     -4.0665260     -1.4730340
H      -0.7275500     -5.6947570     -0.0848900
H       0.0341890     -2.2128640     -2.5364960
H      -0.7126740     -4.6109730     -2.3605770
C      -1.6334250      1.8101530     -0.0502410
H      -2.4144120      2.2075320      0.6167720
H      -1.9974700      1.9396350     -1.0798990
C      -2.3977640     -0.4402980     -0.6162170
H      -2.1405860     -1.4953880     -0.4666060
H      -2.2297380     -0.2013760     -1.6735350
C      -0.3895350      2.6560130      0.0477720
C      -0.4701000      4.0198590      0.3366800
C       1.9077580      2.8314020     -0.3260440
C       0.6841970      4.7981660      0.2793920
H      -1.4343050      4.4592970      0.5952960
C       1.8961370      4.1958400     -0.0702310
H       2.8293630      2.3128270     -0.5923750
H       0.6393370      5.8658970      0.5018210
H       2.8213740      4.7683820     -0.1376890
C      -3.8476400     -0.2116740     -0.2509610
C      -4.4505380     -0.9493940      0.7802460
C      -4.6129800      0.7520420     -0.9256160
C      -5.7786290     -0.7136550      1.1440110
H      -3.8818670     -1.7261150      1.2970340
C      -5.9416280      0.9898540     -0.5647230
H      -4.1706240      1.3162760     -1.7501950
C      -6.5259730      0.2608010      0.4752940
H      -6.2331230     -1.2979190      1.9473410
H      -6.5235820      1.7421760     -1.1019430
H      -7.5653040      0.4442560      0.7572870
N       2.9832080     -0.1921130     -0.2854110
N       0.4298430     -2.0427770     -0.5111650
N       0.7909650      2.0825830     -0.2527640
Mn      0.8008630     -0.0030450     -0.5309140
O       0.8120690      0.0796840     -2.3555120
O      -0.2038590      0.9644160     -2.8183920
H      -0.7141590      0.3881060     -3.4158010
65
Quitnet_MnBnTPEN_Hydroperoxo_G3.log
65
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Final Energy =           -2620.8750989600
C       -2.9809000      -1.5437880       0.6228330
C       -2.7974370      -1.7149820      -1.6909880
C       -3.9148790      -2.5412960      -1.7637320
C       -4.5764600      -2.8738330      -0.5793680
C       -4.1093580      -2.3611890       0.6326420
H       -2.2467190      -1.4245190      -2.5866510
H       -4.2579180      -2.9104580      -2.7306150
H       -5.4580130      -3.5173000      -0.5995230
H       -4.6151950      -2.5831470       1.5730580
C       -2.3892910      -0.9445380       1.8732010
H       -1.6178600      -1.6184820       2.2742050
H       -3.1566490      -0.8208900       2.6530210
N       -1.7452900       0.3560410       1.5530560
C       -0.9103310       0.8576560       2.6813350
H       -1.5316580       1.4371770       3.3803350
H       -0.5511850      -0.0158750       3.2379640
C        0.2565240       1.7051650       2.1997570
H       -0.0973240       2.6205630       1.7081080
H        0.8462290       2.0287590       3.0758880
N        1.0993470       0.9610660       1.2388410
C       -2.7845270       1.3585900       1.1716300
H       -3.2075210       1.8283490       2.0710400
H       -3.6087390       0.8318980       0.6681060
C       -2.2473800       2.3811430       0.2159810
C       -2.7407840       3.6804520       0.1259260
C       -2.2323360       4.5263970      -0.8612070
H       -3.5111820       4.0186350       0.8194630
C       -0.7970480       2.7458960      -1.5804600
C       -1.2493990       4.0514700      -1.7330920
H       -2.6013970       5.5499230      -0.9484260
H       -0.0343150       2.3123870      -2.2300860
H       -0.8317270       4.6812360      -2.5187840
C        1.7929100      -0.1605650       1.9004840
H        1.3345360      -0.3512140       2.8813100
H        2.8426790       0.0775170       2.1113450
C        2.0572590       1.9079510       0.5726240
H        2.4145430       2.6256130       1.3299030
H        1.4856300       2.4828960      -0.1691780
C        1.7088420      -1.4467190       1.1267650
C        2.6788400      -2.4387260       1.2764740
C        0.4345510      -2.8410820      -0.2368490
C        2.4958060      -3.6710380       0.6536740
H        3.5643700      -2.2354050       1.8797730
C        1.3417160      -3.8831740      -0.1046260
H       -0.4587260      -2.9524080      -0.8486060
H        3.2444010      -4.4586360       0.7589750
H        1.1498950      -4.8342010      -0.6018970
C        3.2553410       1.2415520      -0.0609570
C        3.1444650       0.5019820      -1.2473090
C        4.5083630       1.3258730       0.5666480
C        4.2553940      -0.1558040      -1.7804960
H        2.1828090       0.4345460      -1.7510950
C        5.6221050       0.6722800       0.0324530
```

H	4.6119750	1.9055130	1.4877460
C	5.4961410	-0.0773180	-1.1409570
H	4.1470660	-0.7338910	-2.7011260
H	6.5888350	0.7475980	0.5354580
H	6.3637190	-0.5942020	-1.5577740
N	-2.3404960	-1.2407100	-0.5228000
N	-1.2846540	1.9423510	-0.6205230
N	0.6165570	-1.6482030	0.3616710
Mn	-0.5546030	0.0309300	-0.2206210
O	0.0967500	0.0837620	-1.9429360
O	0.4802730	-1.1506600	-2.5160860
H	-0.0686850	-1.1779760	-3.3202740

68

Quitnet_MnBnTPEN_MeCN_G1.log

68

Final Energy =   -2602.5261048400

C	3.3094280	0.0854940	-1.0488870
C	3.5329750	0.1977280	1.2881000
C	4.9144570	0.3055090	1.1922170
C	5.4991840	0.3049500	-0.0761330
C	4.6874650	0.1983650	-1.2073780
H	3.0248220	0.1952820	2.2544090
H	5.5135040	0.3927890	2.0986380
H	6.5813680	0.3947820	-0.1853690
H	5.1139030	0.2051870	-2.2110420
C	2.3619700	-0.0867300	-2.2141720
H	2.2075480	-1.1605590	-2.3973090
H	2.8048280	0.3272800	-3.1332870
N	1.0661420	0.5301600	-1.8939850
C	-0.1033860	-0.0485040	-2.5834720
H	-0.2047980	0.3465750	-3.6078470
H	0.0450230	-1.1319740	-2.6738000
C	-1.3716230	0.2747850	-1.8083740
H	-1.5205890	1.3613500	-1.7840440
H	-2.2430760	-0.1564950	-2.3204880
N	-1.3440950	-0.1957090	-0.3832190
C	1.1274900	2.0047020	-1.9619850
H	0.5436500	2.3799700	-2.8166370
H	2.1666310	2.3132720	-2.1542050
C	0.6881070	2.6991410	-0.6983390
C	0.4885240	4.0796690	-0.6770560
C	0.1625130	4.7077130	0.5221510
H	0.5966750	4.6489220	-1.6011430
C	0.2368690	2.5726230	1.6031450
C	0.0432230	3.9416600	1.6860000
H	0.0044980	5.7871670	0.5511620
H	0.1412370	1.9294360	2.4774950
H	-0.2044200	4.3929840	2.6466420
C	-1.6781870	-1.6436710	-0.2635450
H	-2.5105450	-1.9050490	-0.9307590
H	-2.0263430	-1.8240370	0.7644160
C	-2.2984410	0.6207990	0.4630600
H	-2.0405110	1.6730430	0.3055070
H	-2.0889540	0.3700430	1.5103540

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C       -0.4974000      -2.5371100      -0.4826540
C       -0.6326100      -3.8563260      -0.9062350
C        1.8046800      -2.8314490      -0.1548910
C        0.4937020      -4.6777580      -0.9421360
H       -1.6152460      -4.2306440      -1.1940450
C        1.7293190      -4.1603150      -0.5457940
H        2.7516490      -2.3904490       0.1504700
H        0.4070280      -5.7145110      -1.2715340
H        2.6320570      -4.7709630      -0.5449570
C       -3.7567450       0.3880860       0.1484310
C       -4.3878580       1.0931770      -0.8889820
C       -4.5036470      -0.5407470       0.8896270
C       -5.7286990       0.8533460      -1.1964370
H       -3.8353660       1.8470790      -1.4534950
C       -5.8450180      -0.7810440       0.5837160
H       -4.0382210      -1.0747840       1.7216810
C       -6.4580070      -0.0892830      -0.4650000
H       -6.2069970       1.4100030      -2.0051330
H       -6.4134680      -1.5061510       1.1699770
H       -7.5069790      -0.2763030      -0.7052270
N        2.7605840       0.0870400       0.1901440
N        0.5443470       1.9710140       0.4312010
N        0.7140670      -2.0352030      -0.1397210
Mn       0.7051080      -0.0410250       0.2950590
N        0.2756350      -0.5078250       2.3904040
C        0.0981690      -0.9713010       3.4355150
C       -0.1278000      -1.5485530       4.7409070
H        0.2987800      -2.5622190       4.7697120
H        0.3554440      -0.9232130       5.5061330
H       -1.2095150      -1.5982440       4.9350860
68
Quitnet_MnBnTPEN_MeCN_G2.log
68
Final Energy =          -2602.5214889000
C       -2.4288780       1.9684550      -0.9732470
C       -2.2205690       2.1955590       1.3391730
C       -3.0402870       3.3179010       1.3473620
C       -3.5521100       3.7836500       0.1356060
C       -3.2528920       3.0891950      -1.0367480
H       -1.8089270       1.7968960       2.2639650
H       -3.2711690       3.8080720       2.2932660
H       -4.1962130       4.6641950       0.1051420
H       -3.6658120       3.3981110      -1.9977860
C       -2.1128090       1.1359450      -2.1894530
H       -1.1864610       1.4971890      -2.6621080
H       -2.9163290       1.2375640      -2.9368770
N       -1.9189150      -0.2601300      -1.7668860
C       -1.3005980      -1.1380860      -2.7838320
H       -2.0578540      -1.7704020      -3.2703720
H       -0.8789670      -0.5128120      -3.5796320
C       -0.2376610      -2.0353020      -2.1641120
H       -0.6831290      -2.8162190      -1.5352690
H        0.3237990      -2.5450480      -2.9629600
N        0.7164470      -1.2629710      -1.3136890
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C      -3.1554680      -0.8443840      -1.2140730
H      -3.7583870      -1.3190150      -2.0020790
H      -3.7766000      -0.0447360      -0.7837420
C      -2.8483520      -1.8211350      -0.1186890
C      -3.6918760      -2.8874220       0.1843980
C      -3.3792440      -3.7243310       1.2542700
H      -4.5825150      -3.0539090      -0.4224570
C      -1.4221680      -2.3994930       1.6445670
C      -2.2239770      -3.4743420       1.9983910
H      -4.0272200      -4.5668400       1.5021250
H      -0.5127890      -2.1755510       2.1992850
H      -1.9362720      -4.1028540       2.8410980
C       1.4617880      -0.2742490      -2.1485010
H       0.8077220       0.0771790      -2.9549550
H       2.3227580      -0.7452790      -2.6367520
C       1.6776400      -2.2440350      -0.6556840
H       1.9077430      -3.0042390      -1.4166810
H       1.1265000      -2.7439550       0.1511090
C       1.8571390       0.9126670      -1.3370540
C       3.0189740       1.6462150      -1.5508990
C       1.1568820       2.4110930       0.3259980
C       3.2439610       2.7930820      -0.7910270
H       3.7379540       1.3096990      -2.2969390
C       2.2931190       3.1871070       0.1544540
H       0.4006310       2.6769890       1.0618120
H       4.1552530       3.3758960      -0.9352340
H       2.4276330       4.0812360       0.7629720
C       2.9578240      -1.6218510      -0.1612940
C       3.0347770      -1.0006020       1.0933390
C       4.0983320      -1.6245880      -0.9810980
C       4.1946410      -0.3364770       1.4941980
H       2.1772620      -1.0356980       1.7636320
C       5.2632920      -0.9665430      -0.5821490
H       4.0745060      -2.1390690      -1.9449470
C       5.3081060      -0.3057790       0.6493610
H       4.2286880       0.1535730       2.4693880
H       6.1375490      -0.9679260      -1.2362820
H       6.2150990       0.2190480       0.9567840
N      -1.9040760       1.5497720       0.2017970
N      -1.7271210      -1.5940300       0.6032550
N       0.9513530       1.2949060      -0.4032840
Mn     -0.4877260      -0.0559390       0.0456000
N      -0.0473380       0.2774790       2.1904450
C       0.3679430       0.4230980       3.2600700
C       0.9001330       0.6086640       4.5908880
H       0.7964240       1.6643670       4.8821790
H       0.3493060      -0.0262150       5.3002350
H       1.9645500       0.3289650       4.5953240
68
Quitnet_MnBnTPEN_MeCN_G3.log
68
Final Energy =        -2602.5261051100
C       3.3093940       0.0852210      -1.0487490
C       3.5327680       0.1975400       1.2882550
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C	4.9142640	0.3052400	1.1924720
C	5.4990890	0.3045820	-0.0758300
C	4.6874480	0.1980030	-1.2071330
H	3.0245620	0.1951930	2.2545310
H	5.5132480	0.3925380	2.0989330
H	6.5812860	0.3943500	-0.1849880
H	5.1139640	0.2047750	-2.2107650
C	2.3620080	-0.0869280	-2.2141030
H	2.2074280	-1.1607440	-2.3971880
H	2.8050190	0.3269440	-3.1332070
N	1.0662560	0.5301780	-1.8940690
C	-0.1033310	-0.0483770	-2.5835400
H	-0.2047460	0.3467270	-3.6079050
H	0.0449950	-1.1318550	-2.6738960
C	-1.3715390	0.2750000	-1.8084300
H	-1.5204070	1.3615780	-1.7840610
H	-2.2430290	-0.1561960	-2.3205460
N	-1.3440660	-0.1955510	-0.3832770
C	1.1277810	2.0046890	-1.9620700
H	0.5439510	2.3800310	-2.8166970
H	2.1669500	2.3131520	-2.1543250
C	0.6884820	2.6991710	-0.6984110
C	0.4892090	4.0797470	-0.6770940
C	0.1631790	4.7078120	0.5220920
H	0.5976070	4.6490090	-1.6011470
C	0.2368980	2.5726630	1.6030080
C	0.0435420	3.9417350	1.6858950
H	0.0054090	5.7873010	0.5511310
H	0.1409910	1.9294450	2.4773090
H	-0.2041380	4.3930800	2.6465170
C	-1.6783470	-1.6434880	-0.2636680
H	-2.5107310	-1.9047120	-0.9309060
H	-2.0265520	-1.8238460	0.7642780
C	-2.2983730	0.6210170	0.4630200
H	-2.0404490	1.6732500	0.3054040
H	-2.0888310	0.3703070	1.5103140
C	-0.4976480	-2.5370290	-0.4828010
C	-0.6329830	-3.8562050	-0.9064580
C	1.8043850	-2.8316040	-0.1550070
C	0.4932500	-4.6777530	-0.9423690
H	-1.6156490	-4.2304110	-1.1943140
C	1.7289030	-4.1604520	-0.5459730
H	2.7514030	-2.3907180	0.1503690
H	0.4064730	-5.7144820	-1.2718170
H	2.6315880	-4.7711790	-0.5451440
C	-3.7566900	0.3882990	0.1484820
C	-4.3878350	1.0932420	-0.8890090
C	-4.5035870	-0.5403830	0.8898760
C	-5.7287030	0.8534050	-1.1963500
H	-3.8353640	1.8470430	-1.4536750
C	-5.8449830	-0.7806810	0.5840840
H	-4.0381330	-1.0743040	1.7219890
C	-6.4580060	-0.0890740	-0.4647150
H	-6.2070230	1.4099450	-2.0051120

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H       -6.4134250        -1.5056650         1.1705030
H       -7.5069980        -0.2760910        -0.7048530
N        2.7604520         0.0868250         0.1902460
N        0.5444150         1.9710370         0.4310760
N        0.7138630        -2.0352550        -0.1398070
Mn       0.7049810        -0.0410330         0.2950090
N        0.2756100        -0.5079680         2.3903930
C        0.0982670        -0.9714840         3.4355060
C       -0.1276490        -1.5487690         4.7408930
H        0.2984360        -2.5626490         4.7694850
H        0.3561040        -0.9237490         5.5060580
H       -1.2093390        -1.5979540         4.9353470
63
Quitnet_MnBnTPEN_Oxo_G2.log
63
Final Energy =          -2544.9571014400
C        2.3570430         2.1161010         0.3063570
C        2.0321420         1.9205760        -1.9925350
C        2.8983910         2.9798850        -2.2480320
C        3.5044440         3.6228850        -1.1660790
C        3.2383300         3.1805100         0.1317240
H        1.5301490         1.3841890        -2.8012860
H        3.0935310         3.2888610        -3.2753040
H        4.1905960         4.4556480        -1.3311430
H        3.7126690         3.6457920         0.9965790
C        1.9961390         1.5570730         1.6615600
H        1.1052170         2.0679860         2.0542900
H        2.8115890         1.7135250         2.3841370
N        1.6855650         0.1091500         1.5261690
C        1.0517390        -0.4589020         2.7543460
H        1.8276160        -0.7933920         3.4577790
H        0.5097490         0.3543890         3.2516330
C        0.1083030        -1.6092260         2.4280330
H        0.6441110        -2.4471390         1.9637460
H       -0.3393170        -1.9909630         3.3606810
N       -0.9284240        -1.1364800         1.4833560
C        2.9307520        -0.6363430         1.1692920
H        3.4535820        -0.9577490         2.0806480
H        3.6097490         0.0486190         0.6402860
C        2.6579130        -1.7861770         0.2525510
C        3.5117580        -2.8802440         0.1398440
C        3.2469480        -3.8465420        -0.8307120
H        4.3733140        -2.9637800         0.8028940
C        1.3169560        -2.5851380        -1.4900080
C        2.1383300        -3.6907990        -1.6666610
H        3.9029550        -4.7125320        -0.9352740
H        0.4373130        -2.4082610        -2.1077060
H        1.9040940        -4.4173350        -2.4447990
C       -1.8535710        -0.1715820         2.1099910
H       -1.4588480         0.1396500         3.0870990
H       -2.8273290        -0.6340710         2.3281420
C       -1.6606240        -2.2334400         0.8077520
H       -2.2009080        -2.8560970         1.5387750
H       -0.9310300        -2.8792260         0.2962490
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C        -2.0436170        1.0682040        1.2752090
C        -3.1557010        1.8920640        1.4498070
C        -1.1679100        2.5230020       -0.3275880
C        -3.2569320        3.0681570        0.7103340
H        -3.9294980        1.6036770        2.1621970
C        -2.2401010        3.3926920       -0.1913780
H        -0.3664060        2.7274990       -1.0349620
H        -4.1219410        3.7224880        0.8316870
H        -2.2770370        4.2999220       -0.7944200
C        -2.6298890       -1.6660880       -0.1923230
C        -2.1120560       -0.9722770       -1.3957660
C        -3.9988420       -1.7914610       -0.0410710
C        -3.0781250       -0.2048980       -2.1955820
H        -2.2801250       -1.9055290       -2.0619170
C        -4.8849670       -1.1323660       -0.9122520
H        -4.3988820       -2.3628270        0.7978820
C        -4.4324520       -0.3369660       -1.9785960
H        -2.6719480        0.3866710       -3.0188210
H        -5.9590440       -1.2304890       -0.7402690
H        -5.1460710        0.1859800       -2.6160550
N         1.7649030        1.5126570       -0.7418020
N         1.5702040       -1.6640180       -0.5400690
N        -1.0718330        1.3865210        0.3941990
Mn        0.3308260       -0.0760840       -0.1325560
O        -0.8072270       -0.6163020       -1.4776420
63
Quitnet_MnBnTPEN_Oxo_G3.log
63
Final Energy =         -2544.8823886400
C         3.2534640        0.1724480        0.7095540
C         3.3425230       -0.2475520       -1.6044640
C         4.7290200       -0.3358780       -1.5699350
C         5.3842150       -0.1661770       -0.3482530
C         4.6382490        0.0882500        0.8058020
H         2.7621830       -0.3681150       -2.5198330
H         5.2801260       -0.5373600       -2.4886690
H         6.4718990       -0.2359730       -0.2908790
H         5.1209420        0.2186160        1.7748950
C         2.3504860        0.5050320        1.8713450
H         2.1990010        1.5936450        1.9112950
H         2.8114290        0.2157730        2.8272340
N         1.0393870       -0.1505690        1.6660060
C        -0.1041740        0.5328380        2.3166200
H        -0.1527380        0.3027500        3.3930400
H         0.0372970        1.6161420        2.2288820
C        -1.3970640        0.0837830        1.6524560
H        -1.5457880       -0.9875360        1.8371420
H        -2.2490930        0.6170910        2.0989350
N        -1.3723510        0.2784850        0.1628370
C         1.1087700       -1.5973400        2.0143210
H         0.4209500       -1.8219600        2.8431660
H         2.1130670       -1.8338960        2.3949860
C         0.8213890       -2.5054090        0.8509990
C         0.8045810       -3.8933580        0.9933130
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C       0.5800920      -4.6865620      -0.1296510
H       0.9736560      -4.3367710       1.9754160
C       0.4000470      -2.6918610      -1.4465520
C       0.3806340      -4.0757610      -1.3725620
H       0.5656940      -5.7741410      -0.0387920
H       0.2495030      -2.1406040      -2.3755170
H       0.2104140      -4.6627140      -2.2752640
C      -1.7373140       1.6638440      -0.2467900
H      -2.6223960       2.0168690       0.3015460
H      -1.9912420       1.6317880      -1.3169210
C      -2.2385860      -0.7039680      -0.5609150
H      -1.9807200      -1.7104650      -0.2080310
H      -1.9760160      -0.6281700      -1.6230420
C      -0.5953090       2.6244460      -0.1117730
C      -0.7895260       3.9902980       0.0769560
C       1.7025480       2.9253260      -0.3584390
C       0.3146660       4.8416750       0.0369290
H      -1.7960580       4.3751540       0.2423720
C       1.5793850       4.3006790      -0.2002320
H       2.6740460       2.4687060      -0.5395280
H       0.1876620       5.9157280       0.1821400
H       2.4686430       4.9286100      -0.2561480
C      -3.7188600      -0.4910760      -0.3713370
C      -4.3773130      -0.9621700       0.8187590
C      -4.4747130       0.1841090      -1.3833590
C      -5.7137580      -0.7213470       1.0095530
H      -3.8086790      -1.5194460       1.5626460
C      -5.8116020       0.4283720      -1.1951610
H      -3.9757370       0.5050310      -2.2985150
C      -6.4465980      -0.0189410       0.0075280
H      -6.2250200      -1.0676510       1.9081610
H      -6.3996750       0.9534590      -1.9486910
H      -7.5129820       0.1683830       0.1518260
N       2.6372730       0.0025380      -0.4868890
N       0.6057940      -1.9326500      -0.3489010
N       0.6371350       2.1062430      -0.2945560
Mn      0.6541640       0.0689240      -0.4554570
O       0.3241690       0.0979290      -2.0681480
64
Quitnet_MnBnTPEN_Peroxide_Mn3_G1.log
64
Final Energy =        -2620.4299947200
C       3.3662450      -0.0730020       0.9572820
C       3.8488580      -0.6581060      -1.2400620
C       5.2007750      -0.8244600      -0.9510670
C       5.6359590      -0.5973590       0.3563220
C       4.7043200      -0.2242770       1.3257110
H       3.4471290      -0.8332340      -2.2403410
H       5.8927280      -1.1313130      -1.7363680
H       6.6877940      -0.7215760       0.6218070
H       5.0034420      -0.0583640       2.3618290
C       2.3026370       0.3471520       1.9422510
H       2.1890870       1.4403660       1.8937110
H       2.6252570       0.1111460       2.9723480
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N      1.0159980     -0.2648140      1.6019120
C     -0.1234790      0.4458370      2.1957190
H     -0.2457700      0.1848950      3.2637780
H      0.0875840      1.5218780      2.1590930
C     -1.4237700      0.1369880      1.4714340
H     -1.6445040     -0.9340440      1.5712980
H     -2.2484020      0.6728740      1.9730830
N     -1.3821020      0.4496230      0.0308340
C      1.0194620     -1.7059330      1.9022000
H      0.6038630     -1.9026970      2.9056290
H      2.0661150     -2.0479160      1.9362480
C      0.3258460     -2.5776820      0.8794890
C     -0.2251090     -3.8126460      1.2376810
C     -0.7538590     -4.6322630      0.2409890
H     -0.2338180     -4.1220670      2.2841010
C     -0.1821120     -2.9444660     -1.3587900
C     -0.7251040     -4.1964380     -1.0869330
H     -1.1886750     -5.6003770      0.4981530
H     -0.1704320     -2.5228170     -2.3667050
H     -1.1294690     -4.8064950     -1.8955800
C     -1.5433660      1.8849170     -0.2521440
H     -2.3830510      2.3204840      0.3149340
H     -1.7940060      1.9749840     -1.3204560
C     -2.3949190     -0.3474180     -0.7181210
H     -2.1661530     -1.4047910     -0.5411370
H     -2.2316310     -0.1510320     -1.7850210
C     -0.3025390      2.7199230     -0.0466100
C     -0.3777920      4.0387870      0.4106330
C      1.9875900      2.9104670     -0.3751320
C      0.7869060      4.8051930      0.4626030
H     -1.3389370      4.4540020      0.7175960
C      1.9948980      4.2357140      0.0525520
H      2.9071050      2.4133170     -0.6935410
H      0.7519160      5.8367980      0.8187400
H      2.9272920      4.8012810      0.0692220
C     -3.8367640     -0.0756710     -0.3423850
C     -4.4639910     -0.8178130      0.6710210
C     -4.5727750      0.9310370     -0.9871800
C     -5.7830450     -0.5486490      1.0456310
H     -3.9174040     -1.6241030      1.1665510
C     -5.8919920      1.2041190     -0.6158680
H     -4.1126550      1.5026540     -1.7967160
C     -6.4993700      0.4676240      0.4058670
H     -6.2546870     -1.1383270      1.8353060
H     -6.4493010      1.9904250     -1.1305230
H     -7.5313390      0.6786030      0.6960270
N      2.9593550     -0.2811550     -0.3077780
N      0.3280450     -2.1618520     -0.3949630
N      0.8686100      2.1739580     -0.4115940
Mn     0.8226070     -0.0354010     -0.8565010
O      1.3352480      0.0029550     -2.7047460
O     -0.0458300     -0.0003680     -2.5787480
64
Quitnet_MnBnTPEN_Peroxide_Mn3_G2.log
```

64
Final Energy =   -2620.4299947200
C   3.3662300   -0.0730070   0.9572830
C   3.8488380   -0.6581240   -1.2400580
C   5.2007570   -0.8244650   -0.9510680
C   5.6359450   -0.5973520   0.3563180
C   4.7043070   -0.2242710   1.3257080
H   3.4471060   -0.8332630   -2.2403340
H   5.8927090   -1.1313180   -1.7363700
H   6.6877820   -0.7215600   0.6218000
H   5.0034330   -0.0583470   2.3618240
C   2.3026250   0.3471520   1.9422540
H   2.1890800   1.4403660   1.8937120
H   2.6252460   0.1111450   2.9723500
N   1.0159840   -0.2648090   1.6019190
C   -0.1234900   0.4458500   2.1957210
H   -0.2457880   0.1849100   3.2637800
H   0.0875800   1.5218890   2.1590940
C   -1.4237780   0.1370060   1.4714260
H   -1.6445140   -0.9340260   1.5712810
H   -2.2484140   0.6728910   1.9730700
N   -1.3820980   0.4496470   0.0308260
C   1.0194390   -1.7059270   1.9022160
H   0.6038200   -1.9026810   2.9056400
H   2.0660910   -2.0479110   1.9362880
C   0.3258400   -2.5776830   0.8795000
C   -0.2251050   -3.8126520   1.2376910
C   -0.7538380   -4.6322790   0.2409990
H   -0.2338200   -4.1220690   2.2841130
C   -0.1820930   -2.9444820   -1.3587820
C   -0.7250740   -4.1964590   -1.0869260
H   -1.1886440   -5.6003960   0.4981620
H   -0.1704060   -2.5228380   -2.3666990
H   -1.1294220   -4.8065240   -1.8955740
C   -1.5433560   1.8849450   -0.2521390
H   -2.3830330   2.3205140   0.3149500
H   -1.7940050   1.9750230   -1.3204480
C   -2.3949150   -0.3473860   -0.7181390
H   -2.1661420   -1.4047600   -0.5411730
H   -2.2316320   -0.1509820   -1.7850360
C   -0.3025200   2.7199380   -0.0466110
C   -0.3777530   4.0388010   0.4106360
C   1.9876090   2.9104520   -0.3751500
C   0.7869570   4.8051910   0.4625990
H   -1.3388900   4.4540280   0.7176070
C   1.9949370   4.2356980   0.0525360
H   2.9071150   2.4132900   -0.6935670
H   0.7519830   5.8367960   0.8187390
H   2.9273390   4.8012530   0.0691990
C   -3.8367600   -0.0756520   -0.3423930
C   -4.4639800   -0.8178130   0.6710040
C   -4.5727800   0.9310600   -0.9871720
C   -5.7830340   -0.5486620   1.0456210
H   -3.9173870   -1.6241070   1.1665210

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C      -5.8919970       1.2041290      -0.6158530
H      -4.1126660       1.5026900      -1.7967040
C      -6.4993660       0.4676170       0.4058750
H      -6.2546700      -1.1383550       1.8352890
H      -6.4493120       1.9904380      -1.1304960
H      -7.5313360       0.6785860       0.6960410
N       2.9593360      -0.2811740      -0.3077730
N       0.3280460      -2.1618580      -0.3949540
N       0.8686190       2.1739580      -0.4116050
Mn      0.8225870      -0.0353980      -0.8565020
O       1.3352290       0.0029170      -2.7047500
O      -0.0458500      -0.0003980      -2.5787460
64
Quitnet_MnBnTPEN_Peroxide_Mn3_G3.log
64
Final Energy =         -2620.4287994400
C       2.1946180       2.3317960       0.8105010
C       1.8099070       2.7483660      -1.4397660
C       2.4311680       3.9922200      -1.3682010
C       2.9552010       4.4060830      -0.1417240
C       2.8412230       3.5605940       0.9615180
H       1.3861260       2.3737650      -2.3735390
H       2.5045720       4.6166550      -2.2594350
H       3.4549300       5.3722990      -0.0471900
H       3.2498100       3.8425050       1.9332350
C       1.9940380       1.3918210       1.9738270
H       1.0283390       1.6354950       2.4436290
H       2.7712450       1.5680230       2.7395810
N       1.9525370      -0.0021580       1.5278510
C       1.3599050      -0.9184470       2.5226450
H       2.1384850      -1.5390760       2.9959060
H       0.9264460      -0.3228770       3.3367970
C       0.3053330      -1.8487300       1.9291780
H       0.7803360      -2.6163460       1.3054590
H      -0.2009220      -2.3777510       2.7581240
N      -0.6828400      -1.1507830       1.0808530
C       3.2734980      -0.4538030       1.0725290
H       3.9432440      -0.6616380       1.9256280
H       3.7385470       0.3605810       0.4944110
C       3.1795700      -1.6576730       0.1702860
C       4.1382250      -2.6732650       0.1780740
C       4.0128840      -3.7236150      -0.7330470
H       4.9659080      -2.6371190       0.8882610
C       2.0149780      -2.6813040      -1.5538080
C       2.9337420      -3.7278610      -1.6194010
H       4.7472810      -4.5317710      -0.7466700
H       1.1423890      -2.6214310      -2.2084190
H       2.7979740      -4.5302090      -2.3459930
C      -1.4620010      -0.1660600       1.8561860
H      -0.7881370       0.3253750       2.5700960
H      -2.2490920      -0.6440180       2.4595770
C      -1.5564760      -2.1943970       0.4281150
H      -1.6712410      -3.0284420       1.1404730
H      -1.0043950      -2.5732530      -0.4424500
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C       -2.0453640        0.9064900        0.9718530
C       -3.2900680        1.4901720        1.2163630
C       -1.7191320        2.2305090       -0.9024220
C       -3.7487890        2.4779820        0.3468460
H       -3.8965770        1.1502200        2.0562330
C       -2.9534420        2.8538500       -0.7394520
H       -1.0627920        2.4723690       -1.7413900
H       -4.7254860        2.9398970        0.5049230
H       -3.2840680        3.6108040       -1.4518610
C       -2.9389540       -1.7313810        0.0295440
C       -3.1774030       -1.0619710       -1.1810590
C       -4.0180420       -1.9556300        0.8994040
C       -4.4568280       -0.5994360       -1.4940140
H       -2.3405870       -0.8777800       -1.8560610
C       -5.2983920       -1.4910150        0.5886390
H       -3.8529110       -2.4950500        1.8357600
C       -5.5193410       -0.8035210       -0.6081310
H       -4.6233690       -0.0673550       -2.4336710
H       -6.1240860       -1.6673880        1.2819980
H       -6.5181160       -0.4336430       -0.8521330
N        1.6923340        1.9415430       -0.3729390
N        2.1387150       -1.6764210       -0.6759410
N       -1.2776520        1.2906250       -0.0578160
Mn       0.5556300        0.0203690       -0.5257170
O       -0.2520650       -0.7918590       -2.1113160
O        0.5712390        0.2690660       -2.4298460
65
Triplet_MnBnTPEN_Hydroperoxo_G1.log
65
Final Energy =            -2620.8687140700
C       -3.2823490        0.0199660       -0.8716550
C       -3.4365040       -0.4142270        1.4231400
C       -4.8206870       -0.5340040        1.3439830
C       -5.4408320       -0.3714800        0.1032360
C       -4.6608740       -0.0955700       -1.0227490
H       -2.8876810       -0.5233490        2.3602080
H       -5.3969590       -0.7547520        2.2428440
H       -6.5241700       -0.4658850        0.0095080
H       -5.1107670        0.0259650       -2.0086760
C       -2.3317550        0.3515810       -1.9944710
H       -2.1840130        1.4395470       -2.0489110
H       -2.7259850        0.0303060       -2.9699460
N       -1.0274840       -0.2906330       -1.6937660
C        0.1358310        0.3294030       -2.3780440
H        0.1920340        0.0075550       -3.4296530
H       -0.0013800        1.4173720       -2.3792870
C        1.3986300       -0.0709860       -1.6395740
H        1.5319650       -1.1589560       -1.6955530
H        2.2804080        0.3849400       -2.1126590
N        1.3304180        0.2980850       -0.1910090
C       -1.1136130       -1.7613540       -1.9524740
H       -0.5483510       -2.0195170       -2.8598560
H       -2.1613810       -2.0179210       -2.1662820
C       -0.6708640       -2.5981550       -0.7858070
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C      -0.4830730      -3.9761510      -0.9011510
C      -0.1703360      -4.7124470       0.2395340
H      -0.5904070      -4.4564870      -1.8745410
C      -0.2387030      -2.6746840       1.5040020
C      -0.0572160      -4.0508260       1.4657980
H      -0.0195490      -5.7914660       0.1740610
H      -0.1433470      -2.0941690       2.4220000
H       0.1784240      -4.5898190       2.3837890
C       1.6417990       1.7384690       0.0172300
H       2.4591060       2.0667960      -0.6397600
H       1.9838060       1.8511010       1.0546640
C       2.2741980      -0.5496770       0.6207700
H       1.9966780      -1.5934150       0.4412430
H       2.0641620      -0.3172340       1.6709170
C       0.4410520       2.6261390      -0.1106490
C       0.5592110       3.9944940      -0.3530740
C      -1.8553950       2.8315730       0.2307010
C      -0.5810850       4.7932570      -0.2931330
H       1.5384280       4.4207020      -0.5735950
C      -1.8087520       4.2030820       0.0199760
H      -2.7931120       2.3329940       0.4722400
H      -0.5125250       5.8664760      -0.4797860
H      -2.7228170       4.7922160       0.0958150
C       3.7386390      -0.3447800       0.3115020
C       4.3630650      -1.0732860      -0.7135860
C       4.5022910       0.5764410       1.0451720
C       5.7109160      -0.8664100      -1.0162160
H       3.7962040      -1.8211440      -1.2727610
C       5.8506360       0.7849900       0.7453200
H       4.0428440       1.1291370       1.8681520
C       6.4563720       0.0680980      -0.2908710
H       6.1819590      -1.4425270      -1.8157520
H       6.4308820       1.5045330       1.3272350
H       7.5110840       0.2289860      -0.5253560
N      -2.6975150      -0.1392920       0.3377570
N      -0.5294650      -1.9682800       0.3944360
N      -0.7562690       2.0580790       0.1426870
Mn     -0.6826260       0.0497260       0.3528420
O      -0.5293510       0.0976570       2.1626520
O       0.2251260       1.2099930       2.6707020
H       0.6724970       0.7972230       3.4296260
65
Triplet_MnBnTPEN_Hydroperoxo_G2.log
65
Final Energy =          -2620.8687141800
C       3.2821280       0.0193410       0.8719870
C       3.4366260      -0.4148340      -1.4227870
C       4.8207660      -0.5349130      -1.3433710
C       5.4407100      -0.3725790      -0.1024970
C       4.6605980      -0.0965260       1.0233440
H       2.8879520      -0.5238210      -2.3599580
H       5.3971600      -0.7557460      -2.2421330
H       6.5240100      -0.4672340      -0.0085660
H       5.1103280       0.0248950       2.0093600
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C	2.3314240	0.3512840	1.9946140
H	2.1840280	1.4393000	2.0489760
H	2.7253630	0.0299360	2.9701810
N	1.0270000	-0.2905360	1.6937070
C	-0.1362580	0.3299610	2.3776860
H	-0.1927590	0.0082740	3.4293280
H	0.0012910	1.4178850	2.3788040
C	-1.3990320	-0.0701420	1.6390250
H	-1.5326950	-1.1580650	1.6951360
H	-2.2807790	0.3860830	2.1118800
N	-1.3304590	0.2987040	0.1904150
C	1.1126190	-1.7612620	1.9526290
H	0.5468760	-2.0191670	2.8597840
H	2.1602190	-2.0180770	2.1669440
C	0.6701420	-2.5980850	0.7858680
C	0.4822400	-3.9760600	0.9012610
C	0.1696540	-4.7124070	-0.2394320
H	0.5893720	-4.4563430	1.8747000
C	0.2384160	-2.6747260	-1.5040150
C	0.0567900	-4.0508490	-1.4657530
H	0.0187880	-5.7914120	-0.1739180
H	0.1432960	-2.0942640	-2.4220710
H	-0.1787480	-4.5898730	-2.3837520
C	-1.6413930	1.7391340	-0.0181230
H	-2.4589090	2.0677590	0.6384540
H	-1.9828400	1.8517100	-1.0557510
C	-2.2743270	-0.5489480	-0.6213570
H	-1.9967070	-1.5927050	-0.4420980
H	-2.0644990	-0.3163000	-1.6715030
C	-0.4404520	2.6264730	0.1101970
C	-0.5582250	3.9948060	0.3528940
C	1.8561280	2.8312360	-0.2306500
C	0.5823470	4.7932150	0.2933710
H	-1.5373490	4.4212820	0.5733080
C	1.8098810	4.2027190	-0.0196290
H	2.7937330	2.3324300	-0.4721480
H	0.5140880	5.8664120	0.4802620
H	2.7241510	4.7915750	-0.0951510
C	-3.7387220	-0.3442610	-0.3117020
C	-4.3629850	-1.0737660	0.7127730
C	-4.5024900	0.5777110	-1.0443070
C	-5.7107820	-0.8671860	1.0158470
H	-3.7960160	-1.8221620	1.2711250
C	-5.8507780	0.7859780	-0.7440050
H	-4.0432070	1.1312290	-1.8668180
C	-6.4563510	0.0680560	0.2915690
H	-6.1816860	-1.4440950	1.8148940
H	-6.4311090	1.5061140	-1.3251010
H	-7.5110210	0.2287220	0.5263940
N	2.6974840	-0.1397760	-0.3375370
N	0.5290540	-1.9682760	-0.3944450
N	0.7567380	2.0580780	-0.1430200
Mn	0.6826520	0.0496840	-0.3529960
O	0.5297390	0.0974830	-2.1628330

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O          -0.2244360          1.2098820         -2.6711720
H          -0.6718260          0.7970640         -3.4300580
65
Triplet_MnBnTPEN_Hydroperoxo_G3.log
65
Final Energy =            -2620.8614712300
C          -3.2301170         -0.3508450         -0.0657080
C          -2.4575660          0.3613010         -2.1542970
C          -3.7573300          0.4503300         -2.6444150
C          -4.8206530          0.1314010         -1.7988210
C          -4.5532340         -0.2701740         -0.4876020
H          -1.5892170          0.5890910         -2.7711310
H          -3.9245270          0.7720760         -3.6726460
H          -5.8509020          0.2006630         -2.1523850
H          -5.3586660         -0.5163750          0.2049140
C          -2.8080560         -0.8132380          1.3035300
H          -2.5901610         -1.8906650          1.2783030
H          -3.6029110         -0.6650340          2.0491390
N          -1.5656480         -0.0941970          1.6812130
C          -0.7481980         -0.8061740          2.6969970
H          -1.1810270         -0.6896750          3.7030130
H          -0.7577600         -1.8765280          2.4626230
C           0.6530900         -0.2304950          2.6652330
H           0.6222930          0.8214440          2.9791610
H           1.3022960         -0.7564730          3.3820710
N           1.2687870         -0.2629610          1.2977000
C          -1.8744070          1.3073270          2.1049430
H          -1.5713130          1.4546320          3.1513970
H          -2.9638730          1.4554090          2.0878660
C          -1.2432680          2.3515180          1.2261470
C          -1.4105100          3.7144380          1.4806270
C          -0.8741420          4.6400290          0.5889860
H          -1.9662650          4.0353180          2.3627440
C          -0.0599250          2.8092310         -0.7275670
C          -0.1986010          4.1780740         -0.5447080
H          -0.9930180          5.7100920          0.7681050
H           0.4421740          2.3823640         -1.5954130
H           0.2171110          4.8661930         -1.2811260
C           1.8501030         -1.5934970          1.0015520
H           2.4225260         -1.9790260          1.8597630
H           2.5574500         -1.4665170          0.1699230
C           2.3452220          0.8114560          1.3049770
H           2.8263110          0.7656610          2.2944410
H           1.8207750          1.7723910          1.2427610
C           0.8357840         -2.5935550          0.5381210
C           1.0448540         -3.9683920          0.6474020
C          -1.1202120         -2.9345780         -0.6823930
C           0.1302080         -4.8399120          0.0588240
H           1.9205800         -4.3416220          1.1793020
C          -0.9650140         -4.3132260         -0.6312800
H          -1.9603380         -2.4836700         -1.2086580
H           0.2733320         -5.9195710          0.1314780
H          -1.6959810         -4.9577120         -1.1197670
C           3.4251040          0.7246470          0.2567760
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C       3.3241130        1.4114540       -0.9606170
C       4.5940780       -0.0122020        0.5158490
C       4.3468210        1.3405820       -1.9089570
H       2.4434690        2.0147510       -1.1666690
C       5.6166120       -0.0909770       -0.4315100
H       4.7068510       -0.5294780        1.4719950
C       5.4922520        0.5821150       -1.6508820
H       4.2494640        1.8845760       -2.8511500
H       6.5153400       -0.6720330       -0.2132570
H       6.2918410        0.5251790       -2.3930850
N      -2.2090860       -0.0368760       -0.8967310
N      -0.5514660        1.9200990        0.1569990
N      -0.2481440       -2.0968050       -0.0904880
Mn     -0.3806290       -0.0832730       -0.0577690
O       0.6429630        0.1063480       -1.5374640
O       0.3679540       -0.8575190       -2.5649420
H       0.7394040       -0.3989200       -3.3383260
68
Triplet_MnBnTPEN_MeCN_G2.log
68
Final Energy =          -2602.5164252900
C      -3.2829800       -0.1091720       -1.0188360
C      -3.4485870       -0.3709620        1.3071950
C      -4.8304760       -0.4951520        1.2284930
C      -5.4443460       -0.4227770       -0.0236430
C      -4.6594680       -0.2325400       -1.1636740
H      -2.9262350       -0.4235510        2.2622490
H      -5.4093760       -0.6492430        2.1391350
H      -6.5272860       -0.5223090       -0.1147760
H      -5.1040950       -0.1849300       -2.1580520
C      -2.3349480        0.1372420       -2.1594280
H      -2.2048110        1.2172450       -2.3154270
H      -2.7109050       -0.2809660       -3.1038620
N      -1.0209270       -0.4532920       -1.7915240
C       0.1271330        0.1513510       -2.5293130
H       0.1705160       -0.2394070       -3.5568680
H      -0.0388550        1.2325070       -2.5995300
C       1.4025880       -0.1745220       -1.7828750
H       1.5776850       -1.2571510       -1.7969400
H       2.2665140        0.2991090       -2.2689790
N       1.3171770        0.2455580       -0.3433540
C      -1.0717010       -1.9440580       -1.9543960
H      -0.5382600       -2.2421030       -2.8674140
H      -2.1208080       -2.2412690       -2.0996340
C      -0.5597200       -2.6791330       -0.7529310
C      -0.2749930       -4.0426700       -0.7845760
C       0.0784280       -4.6853150        0.4007220
H      -0.3405520       -4.5876570       -1.7267520
C      -0.1389690       -2.5909070        1.5467760
C       0.1337080       -3.9497970        1.5885380
H       0.3049080       -5.7528740        0.3993450
H      -0.0868120       -1.9748370        2.4427190
H       0.3965790       -4.4171700        2.5374130
C       1.6174470        1.6961630       -0.1738750
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H        2.4557960        1.9968540       -0.8164050
H        1.9439000        1.8484040        0.8650250
C        2.2813190       -0.5676360        0.4962720
H        2.0479380       -1.6207740        0.3133570
H        2.0550880       -0.3425610        1.5452100
C        0.4190890        2.5689980       -0.3850870
C        0.5360440        3.9262220       -0.6784220
C       -1.8959420        2.7635720       -0.1560350
C       -0.6126460        4.7145990       -0.7031640
H        1.5209640        4.3518530       -0.8720560
C       -1.8477840        4.1244770       -0.4220610
H       -2.8406600        2.2706720        0.0647540
H       -0.5450070        5.7796820       -0.9308200
H       -2.7699630        4.7054140       -0.4123030
C        3.7385290       -0.3025390        0.2031380
C        4.4588420        0.6327520        0.9624900
C        4.3985190       -0.9905980       -0.8276940
C        5.8009640        0.8963740        0.6804130
H        3.9720390        1.1529450        1.7910350
C        5.7402100       -0.7274360       -1.1119070
H        3.8678830       -1.7504460       -1.4051910
C        6.4422520        0.2215020       -0.3624680
H        6.3481970        1.6258850        1.2812380
H        6.2405180       -1.2713290       -1.9159660
H        7.4921390        0.4262220       -0.5835010
N       -2.7001890       -0.1746450        0.2061510
N       -0.4664730       -1.9711560        0.3930020
N       -0.7845280        1.9991010       -0.1602280
Mn      -0.7036380       -0.0037620        0.1669080
N       -0.4441690        0.4440200        2.0746680
C       -0.3078720        0.8289920        3.1558010
C       -0.1271000        1.3007140        4.5086580
H       -0.7504060        2.1915120        4.6752030
H       -0.4194910        0.5063700        5.2116310
H        0.9323210        1.5543890        4.6637580
63
Triplet_MnBnTPEN_Oxo_G1.log
63
Final Energy =          -2544.9006074300
C        2.6303430        1.3627860       -0.3437130
C        1.9140400        0.3187580       -2.3307920
C        3.0648280        0.7217920       -2.9970890
C        4.0220860        1.4623400       -2.2999270
C        3.8038250        1.7846000       -0.9574820
H        1.1253230       -0.2585450       -2.8151230
H        3.2018450        0.4531660       -4.0445180
H        4.9386510        1.7852760       -2.7964630
H        4.5353650        2.3565520       -0.3860740
C        2.2528260        1.6934770        1.0768790
H        1.6464350        2.6105980        1.0938200
H        3.1419950        1.8840700        1.6945580
N        1.4422140        0.5732370        1.6135410
C        0.5454810        0.9223380        2.7465020
H        1.1039400        0.9683010        3.6932890
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H        0.1236680        1.9200800        2.5766260
C       -0.5280710       -0.1452100        2.8143300
H       -0.0863780       -1.1369260        2.9765230
H       -1.2222140        0.0384250        3.6463290
N       -1.2929010       -0.1904450        1.5206060
C        2.3186620       -0.5791610        1.9834220
H        2.2350510       -0.7864730        3.0592150
H        3.3687980       -0.2996850        1.8165180
C        2.0412910       -1.8128230        1.1829860
C        2.7578270       -2.9907840        1.3947190
C        2.5820930       -4.0592450        0.5204430
H        3.4634100       -3.0462500        2.2244870
C        1.0212480       -2.7220370       -0.7107880
C        1.7189980       -3.9096710       -0.5704320
H        3.1349360       -4.9884710        0.6682950
H        0.3716390       -2.5378830       -1.5629380
H        1.5882860       -4.6989240       -1.3106810
C       -2.2289870        0.9758100        1.4496770
H       -2.5833370        1.2333420        2.4575330
H       -3.1108040        0.6761930        0.8710110
C       -2.0837270       -1.4829010        1.4498710
H       -2.7495290       -1.5112060        2.3249730
H       -1.3642590       -2.3063870        1.5426320
C       -1.6575070        2.1551420        0.7382530
C       -2.2362310        3.4199040        0.8356110
C       -0.1936960        2.8943810       -0.9215150
C       -1.7663570        4.4433170        0.0171620
H       -3.0548090        3.5838810        1.5370870
C       -0.7395130        4.1684420       -0.8900880
H        0.6075460        2.6525640       -1.6145110
H       -2.2038140        5.4412650        0.0762570
H       -0.3542010        4.9305400       -1.5673190
C       -2.8736770       -1.5837690        0.1789220
C       -4.2102780       -1.2238820        0.1025510
C       -2.1984840       -1.9922890       -1.0191350
C       -4.8722980       -1.2058720       -1.1413520
H       -4.7586480       -0.9446790        1.0043810
C       -2.8818750       -1.9641190       -2.2751930
H       -1.3756840       -2.6945400       -0.9099490
C       -4.1982990       -1.5577300       -2.3308270
H       -5.9204880       -0.9040010       -1.1829430
H       -2.3493800       -2.2875200       -3.1707630
H       -4.7312440       -1.5358730       -3.2825440
N        1.7172040        0.6389770       -1.0395030
N        1.1414470       -1.7153130        0.1834140
N       -0.6290900        1.9144620       -0.1003900
Mn       0.1252820        0.0229580        0.0035760
O       -0.8166950       -0.5348530       -1.2713480
63
Triplet_MnBnTPEN_Oxo_G2.log
63
Final Energy =          -2544.9006072200
C        2.6305860        1.3625510       -0.3436870
C        1.9141460        0.3187780       -2.3308630
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C      3.0650620      0.7215820     -2.9970740
C      4.0224400      1.4618920     -2.2998290
C      3.8041810      1.7841460     -0.9573790
H      1.1253200     -0.2583320     -2.8152440
H      3.2020700      0.4530030     -4.0445170
H      4.9391120      1.7846240     -2.7963010
H      4.5358070      2.3559320     -0.3859100
C      2.2530580      1.6932710      1.0768980
H      1.6466470      2.6103860      1.0938000
H      3.1422180      1.8838640      1.6945890
N      1.4424190      0.5730540      1.6135410
C      0.5457390      0.9221020      2.7465420
H      1.1041920      0.9678260      3.6933450
H      0.1241060      1.9199540      2.5768460
C     -0.5279980     -0.1452840      2.8142560
H     -0.0864650     -1.1370790      2.9763940
H     -1.2221060      0.0384070      3.6462750
N     -1.2928850     -0.1903990      1.5205530
C      2.3187970     -0.5794450      1.9832490
H      2.2354710     -0.7866660      3.0590800
H      3.3689300     -0.3001410      1.8160190
C      2.0410310     -1.8131050      1.1829510
C      2.7571450     -2.9913010      1.3948030
C      2.5811480     -4.0597250      0.5205330
H      3.4626240     -3.0469930      2.2246460
C      1.0209340     -2.7220200     -0.7109500
C      1.7182620     -3.9098890     -0.5704750
H      3.1336560     -4.9891350      0.6684870
H      0.3715240     -2.5376420     -1.5632090
H      1.5873790     -4.6991200     -1.3107160
C     -2.2288670      0.9759480      1.4497630
H     -2.5830680      1.2334480      2.4576780
H     -3.1107700      0.6764520      0.8711770
C     -2.0837620     -1.4827640      1.4497900
H     -2.7495590     -1.5110910      2.3249010
H     -1.3643760     -2.3063370      1.5424940
C     -1.6573620      2.1552570      0.7383280
C     -2.2360850      3.4200260      0.8356500
C     -0.1933750      2.8945260     -0.9212810
C     -1.7661260      4.4434470      0.0172650
H     -3.0547340      3.5840000      1.5370490
C     -0.7391680      4.1685970     -0.8898660
H      0.6079570      2.6527230     -1.6141710
H     -2.2035820      5.4413970      0.0763410
H     -0.3537610      4.9307130     -1.5670220
C     -2.8738270     -1.5835720      0.1788660
C     -2.1988120     -1.9921710     -1.0192360
C     -4.2103810     -1.2234920      0.1025740
C     -2.8822200     -1.9638530     -2.2752390
H     -1.3758810     -2.6942720     -0.9101660
C     -4.8724730     -1.2053610     -1.1412920
H     -4.7586550     -0.9441760      1.0044250
C     -4.1985960     -1.5572720     -2.3308080
H     -2.3497920     -2.2872740     -3.1708410
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H        -5.9206230        -0.9033420        -1.1828100
H        -4.7315890        -1.5352910        -3.2824960
N         1.7173130         0.6389750        -1.0395660
N         1.1413370        -1.7153390         0.1832670
N        -0.6288970         1.9145830        -0.1002450
Mn        0.1253850         0.0230640         0.0034990
O        -0.8165690        -0.5344720        -1.2714270
63
Triplet_MnBnTPEN_Oxo_G3.log
63
Final Energy =            -2544.8917261600
C         3.2517060        -0.0077210         0.7838250
C         3.3845270        -0.5329300        -1.5163320
C         4.7598770        -0.6967550        -1.4274560
C         5.3875110        -0.5079320        -0.1939650
C         4.6237280        -0.1640060         0.9251280
H         2.8473320        -0.6638230        -2.4557650
H         5.3234620        -0.9688170        -2.3199450
H         6.4673020        -0.6343040        -0.0998270
H         5.0818310        -0.0206840         1.9040610
C         2.3234160         0.3964600         1.8931360
H         2.2293830         1.4906150         1.9290840
H         2.6996300         0.0762160         2.8743710
N         0.9920800        -0.1987020         1.6048340
C        -0.1426910         0.5122760         2.2561200
H        -0.2130650         0.2438940         3.3206940
H         0.0446430         1.5906510         2.2061820
C        -1.4128380         0.1245810         1.5329280
H        -1.6134100        -0.9458220         1.6577790
H        -2.2770450         0.6669490         1.9377450
N        -1.3004190         0.3865750         0.0541500
C         1.0079060        -1.6578850         1.9414400
H         0.4314320        -1.8415630         2.8588680
H         2.0417720        -1.9572200         2.1676250
C         0.5256300        -2.5174130         0.8150440
C         0.2518870        -3.8728980         0.9799220
C        -0.0761550        -4.6390810        -0.1373190
H         0.3112830        -4.3152770         1.9748570
C         0.1350200        -2.6758430        -1.4983100
C        -0.1215340        -4.0330030        -1.3973080
H        -0.2907810        -5.7034200        -0.0279380
H         0.0917340        -2.1471280        -2.4501540
H        -0.3646400        -4.5997540        -2.2959860
C        -1.5475190         1.8229950        -0.2850240
H        -2.3946740         2.2052570         0.2980630
H        -1.8284260         1.8692130        -1.3465990
C        -2.2654730        -0.4969480        -0.7292070
H        -2.0120500        -1.5313230        -0.4839410
H        -2.0450120        -0.3224670        -1.7914760
C        -0.3306980         2.6718900        -0.1207950
C        -0.3999180         4.0465200         0.0816770
C         1.9946860         2.7726110        -0.3724850
C         0.7757340         4.7958970         0.0476890
H        -1.3689880         4.5164860         0.2505280
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C      1.9883480        4.1495870       -0.2012680
H      2.9232350        2.2403200       -0.5659690
H      0.7438950        5.8753590        0.2036290
H      2.9290180        4.6970450       -0.2584370
C     -3.7122040       -0.2320220       -0.4165380
C     -4.3619740       -0.9665990        0.5914410
C     -4.4398880        0.7335290       -1.1356590
C     -5.7004950       -0.7209130        0.8940640
H     -3.8221610       -1.7460950        1.1334040
C     -5.7794370        0.9766000       -0.8352790
H     -3.9644980        1.2843610       -1.9497060
C     -6.4099500        0.2561460        0.1856490
H     -6.1949250       -1.2977500        1.6780460
H     -6.3361810        1.7237070       -1.4042060
H     -7.4590230        0.4474480        0.4211800
N      2.6620350       -0.1900470       -0.4287870
N      0.4401840       -1.9404680       -0.4040300
N      0.8568980        2.0513270       -0.3064140
Mn     0.6909880        0.0368070       -0.4882160
O      0.3666970        0.1080120       -2.0957180
64
Triplet_MnBnTPEN_Peroxide_Mn3_G1.log
64
Final Energy =           -2620.3908182000
C      3.3037900        0.1210120        1.0603340
C      3.7679700       -0.5326650       -1.1126930
C      5.1312210       -0.6385100       -0.8392540
C      5.5790920       -0.3405270        0.4505900
C      4.6504820        0.0384610        1.4215190
H      3.3486150       -0.7595700       -2.0955160
H      5.8239320       -0.9534130       -1.6211320
H      6.6393180       -0.4148310        0.7014930
H      4.9590510        0.2594890        2.4448400
C      2.2132880        0.5233440        2.0211230
H      2.0609470        1.6122090        1.9629470
H      2.5047070        0.2979600        3.0619270
N      0.9542270       -0.1372180        1.6474360
C     -0.2065750        0.5044770        2.2827500
H     -0.2675970        0.2561130        3.3578890
H     -0.0741990        1.5925190        2.2160750
C     -1.4852660        0.0765180        1.5935590
H     -1.6244600       -1.0048430        1.7254960
H     -2.3504390        0.5669810        2.0686030
N     -1.4470880        0.3464290        0.1404960
C      1.0207420       -1.5945820        1.9041710
H      0.4220910       -1.8606420        2.7907210
H      2.0578480       -1.8591430        2.1619210
C      0.6261590       -2.4756620        0.7403940
C      0.4339410       -3.8476940        0.9265020
C      0.1657220       -4.6559000       -0.1767400
H      0.5022050       -4.2699960        1.9303760
C      0.2889870       -2.6991670       -1.5578690
C      0.1027940       -4.0713620       -1.4450680
H      0.0112020       -5.7291520       -0.0495920
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H      0.2414540      -2.1709570      -2.5101990
H     -0.0945110      -4.6673860      -2.3369480
C     -1.7217830       1.7651110      -0.1820800
H     -2.5343360       2.1761370       0.4372410
H     -2.0620810       1.7983350      -1.2274850
C     -2.3938990      -0.5555470      -0.5887470
H     -2.0930340      -1.5840310      -0.3540130
H     -2.2185490      -0.4008580      -1.6599110
C     -0.5046410       2.6491340      -0.1209450
C     -0.5844920       4.0111420       0.1710190
C      1.7719200       2.8297990      -0.5906530
C      0.5670050       4.7937710       0.0720080
H     -1.5397410       4.4472380       0.4662060
C      1.7649950       4.1960880      -0.3266420
H      2.6773540       2.3079440      -0.9006460
H      0.5281230       5.8608090       0.2997150
H      2.6838820       4.7743090      -0.4290260
C     -3.8550600      -0.3563080      -0.2501900
C     -4.4502390      -1.0588010       0.8100010
C     -4.6452980       0.5422130      -0.9845120
C     -5.7913660      -0.8524520       1.1430730
H     -3.8621070      -1.7853920       1.3756480
C     -5.9867580       0.7522320      -0.6545320
H     -4.2106330       1.0772930      -1.8322310
C     -6.5621520       0.0587500       0.4145010
H     -6.2373660      -1.4098540       1.9700970
H     -6.5859260       1.4545860      -1.2387090
H     -7.6114240       0.2201000       0.6725250
N      2.8850970      -0.1511550      -0.1816280
N      0.5306390      -1.9234260      -0.4836160
N      0.6659450       2.0784760      -0.4697940
Mn     0.6075690       0.0729770      -0.6618480
O      1.2871850       0.0807190      -2.4976130
O     -0.1132800       0.1386060      -2.3151460
64
Triplet_MnBnTPEN_Peroxide_Mn3_G2.log
64
Final Energy =        -2620.3908182700
C      3.3031800       0.1215350       1.0604020
C      3.7669240      -0.5319760      -1.1127850
C      5.1301870      -0.6381300      -0.8395340
C      5.5783140      -0.3403850       0.4502600
C      4.6498960       0.0386700       1.4213490
H      3.3474220      -0.7587100      -2.0955730
H      5.8226930      -0.9531180      -1.6215590
H      6.6385550      -0.4149270       0.7010240
H      4.9586410       0.2594960       2.4446590
C      2.2128890       0.5237540       2.0214620
H      2.0603110       1.6125840       1.9632260
H      2.5046830       0.2985030       3.0621940
N      0.9539410      -0.1370740       1.6480800
C     -0.2070400       0.5044620       2.2831180
H     -0.2682510       0.2562460       3.3582840
H     -0.0748420       1.5925250       2.2163280
```

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C     -1.4854750      0.0762070      1.5936520
H     -1.6243660     -1.0052130      1.7254410
H     -2.3509060      0.5663670      2.0685260
N     -1.4470590      0.3462240      0.1406020
C      1.0206220     -1.5944030      1.9046620
H      0.4214000     -1.8607080      2.7907590
H      2.0575840     -1.8588070      2.1631590
C      0.6269390     -2.4755320      0.7405710
C      0.4355850     -3.8477080      0.9265220
C      0.1678850     -4.6559950     -0.1767800
H      0.5041060     -4.2700450      1.9303660
C      0.2900080     -2.6990690     -1.5577300
C      0.1046060     -4.0713710     -1.4450510
H      0.0140370     -5.7293550     -0.0497300
H      0.2422840     -2.1708320     -2.5100340
H     -0.0923210     -4.6674210     -2.3369980
C     -1.7218700      1.7649020     -0.1818340
H     -2.5344750      2.1758070      0.4375020
H     -2.0621710      1.7982370     -1.2272390
C     -2.3937210     -0.5557850     -0.5887980
H     -2.0927140     -1.5842510     -0.3541520
H     -2.2183150     -0.4009830     -1.6599330
C     -0.5048250      2.6490540     -0.1206640
C     -0.5847860      4.0110200      0.1715100
C      1.7715920      2.8300910     -0.5909600
C      0.5665770      4.7938060      0.0722690
H     -1.5400120      4.4469480      0.4670120
C      1.7645370      4.1963530     -0.3268350
H      2.6770000      2.3083790     -0.9012530
H      0.5276260      5.8608090      0.3001360
H      2.6832900      4.7747420     -0.4294690
C     -3.8549280     -0.3567580     -0.2503410
C     -4.4501270     -1.0593930      0.8097500
C     -4.6452280      0.5416830     -0.9846960
C     -5.7913120     -0.8532380      1.1427060
H     -3.8619510     -1.7859360      1.3754110
C     -5.9867460      0.7515150     -0.6548290
H     -4.2105620      1.0768550     -1.8323560
C     -6.5621500      0.0579070      0.4141170
H     -6.2373160     -1.4107470      1.9696560
H     -6.5859490      1.4538160     -1.2390320
H     -7.6114680      0.2191000      0.6720480
N      2.8842200     -0.1503570     -0.1815690
N      0.5311610     -1.9232400     -0.4833990
N      0.6657490      2.0786050     -0.4698250
Mn     0.6077990      0.0730970     -0.6620150
O      1.2868570      0.0810460     -2.4978680
O     -0.1136400      0.1385580     -2.3151710


6
Methanol.log
6
Final Energy =          -115.7676644360
C      0.6570980     -0.0191380      0.0000010
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H          1.0969670          0.9904910         -0.0007480
H          1.0376680         -0.5498310         -0.8946250
H          1.0378020         -0.5485630          0.8953310
O         -0.7475310          0.1231490          0.0000030
H         -1.1347790         -0.7624570          0.0000120
69
```