

Supporting Information Materials

Reactivity of Superoxide Radical Anion with Cyclic Nitrones: Role of Intramolecular H-Bond and Electrostatic Effects

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Table S1. Comparison of Selected X-ray Crystallographic Bond Lengths with Calculated Bond Lengths (B3LYP/6-31G*).

Bonds	Calculated Bond	Experimental Bond
	Distances Range ^a (Å)	Distances (Å)
Nitronyl C=N	1.30-1.31	1.291(2), ² 1.307(2) ³
Nitronyl N-O	1.25-1.27	1.2987(16); ² 1.294(1) ³
Nitroxyl C-N	1.47-1.49	1.50 ⁴
Nitroxyl N-O	1.27-1.28	1.27 ⁴
P=O	1.47-1.49	1.4636(12); ² 1.458(2) ⁵
P-OEt	1.59-1.62	1.580(1); ² 1.575(2) ⁵
P-C _{ring}	1.80-1.88	1.8276(16); ² 1.813(3) ⁵
C=O	1.20-1.22	1.233(5) ⁶
C(O)-OEt	1.33-1.35	1.358(5) ⁶
C(O)-C _{ring}	1.53-1.56	1.506(5) ⁶
MeS=O	1.46-1.47	1.435(2) ⁷
S-CH ₃	1.81-1.82	1.755(3) ⁷
SO ₂ -C _{ring}	1.89-1.93	1.833(2) ⁸
C _{ring} -CF ₃	1.53-1.55	1.530(3) ³
C(O)-NH ₂	1.32-1.36 ^b	1.32-1.33 ⁹
C(O)-NHCH ₃	1.31-1.38 ^b	1.33 ¹⁰
C(O)-N(CH ₃) ₂	1.36-1.38 ^b	1.33 ¹¹
N _{amide} -CH ₃	1.44-1.47	1.46 ^{10,11}
C _{ring} -O ₂ ⁻	1.37-1.43	1.44 ¹²
O-O ⁻	1.40-1.48	1.40; ¹³ 1.46 ¹⁴
C _{ring} -O ₂ H	1.41-1.42	1.44 ¹²
	1.45-1.46	1.46 ¹²

^a For certain functional groups other than the nitronyl and nitroxyl groups, values are based on both nitrones and spin adducts. ^bBond lengths for amide C(O)-N is lowest in O₂ adducts while O₂H anmd nitrones are the same.

A. Tautomerization. To test if the high C-2 charge densities observed for the amido-nitrones is exclusively a contribution from the amido tautomers and not from the imidic form, conformational as well as configurational searches for the most stable structure were carried out on the imidic forms of AMPO, MAMPO, and DiMAPO. Of all the optimized conformational and configurational isomers, the *Z*-isomer with a conformation that exhibits strong intramolecular H-bonding interaction between with the nitronyl-O and hydroxyl-H were predicted to be the most stable forms for AMPO, MAMPO and DiMAPO (see Figure 1 for MAMPO). The calculated C-2 charge density for the most preferred imidic acid forms are 0.046 e, 0.041 e and 0.077 e for AMPO, MAMPO and DiMAPO, respectively, which are less positive compared to the C-2 charge observed for their respective amide tautomers (see Table 1 of main text). The lactim form of spirolactam-nitrone, TAMPO, gave a conformation in which the hydroxyl-H does not exhibit intramolecular H-bonding with the nitronyl-O and is more preferred by $\Delta G_{(aq)} = 6.1$ kcal/mol in solution than its *E*-isomer that exhibits intramolecular H-bonding. The lactim *E*-isomer has a C-2 charge of -0.004 e with a calculated free energy difference for lactam-lactim equilibrium of $\Delta G_{(aq)} = -23.6$ kcal/mol with $K \sim 10^{-18}$ which indicates that the lactim form is even less favored in solution than the formation of imidic acid form. Hence, based on the calculated equilibrium constants, the contribution of the imidic acid and lactim tautomeric forms in solution should be insignificant and that the amide forms should dominate in solution.

B. Calculated Isotropic Hyperfine Splitting Constants. In order to justify the DFT approach employed in this study, the electron spin distribution within the nitrone-O₂H adducts was assessed from the calculated isotropic hyperfine splitting constant (hfsc), $a_{(X)}$, which is directly proportional to the nuclear spin density ρ_{rx} based on the equation (1),

$$a_X = 8\pi/3(g_e/g_0)\gamma_x\beta_x\rho_{rx} \quad (1)$$

where g_0 is the isotropic g-value for the radical, g_e the g-value for the free electron, γ_x the gyromagnetic nuclear ratio, and β_x the nuclear magneton of the nucleus X.¹⁵

The calculated hfsc's in the gas phase at the B3LYP level for the four model adducts, i.e., AMPO-O₂H, DMPO-O₂H, EMPO-O₂H and DEPMPO-O₂H were compared with their respective experimental hfsc's in aqueous and DMSO solutions as shown in Table S2 (also see Figure S1 for the simulated spectra). We have reasonably predicted the hfsc's of the relevant nuclei and shown that the Boltzmann-averaged values are in good agreement with the experimental values. As we have demonstrated previously for DMPO-O₂H,¹⁶ the accuracy of the theoretical gas phase hfsc values can be improved by considering the explicit interaction of water molecules with the adduct as well as the bulk dielectric effect of the solvent. We also found that accuracy of the hfsc values predicted using the 6-31+G** basis set is comparable other basis sets previously considered.¹⁶ Other factors that were not considered and may also influence the hfcc values are dynamic effects induced by the low-frequency inversion motion on the nitrogen atom (an error of approximately 1G),¹⁷ and perhaps due to the exchange interaction from neighboring adducts as we discussed in our previous work.¹⁶

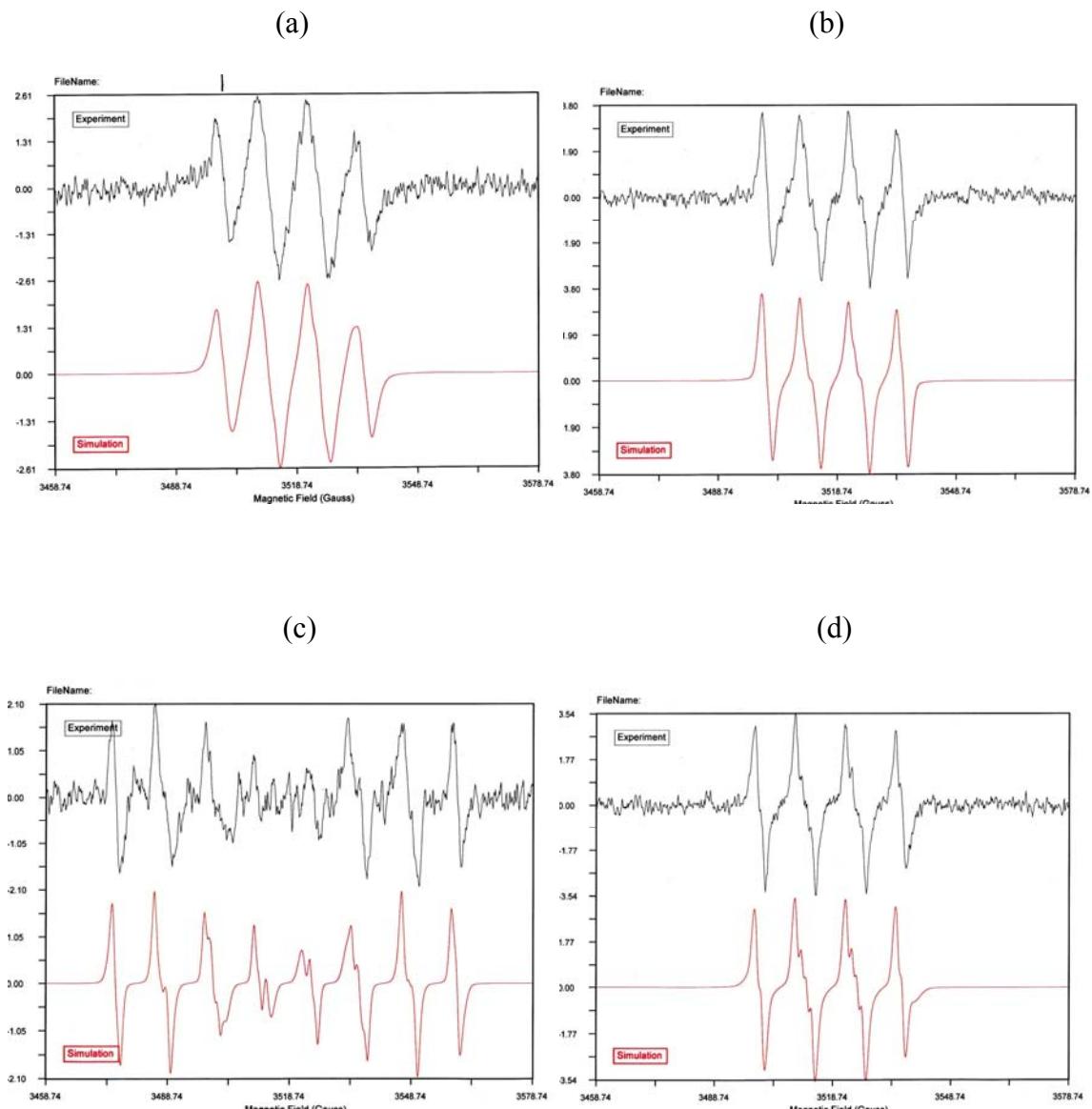


Figure S1. X-band EPR spectra of the superoxide radical anion adducts of (a) AMPO; (b) EMPO; (c) DEPMPO; (d) DMPO in 5% water-95% DMF solution with saturated KO₂. Spectrometric setting: Scan Range: 120 G; MA: 0.5 G; MF: 100 kHz; TC: 81.9 ms; RG: 3.5 x 10⁵; MW power: 19.85 mW.

Table S2. Calculated (gas) and Experimental (aqueous and DMSO) Isotropic Hyperfine Splitting Constants of Selected Atoms at the B3LYP/6-31+G**/B3LYP6-31G* Level of Theory.^a

Isotropic Hyperfine Splitting Constants (G)				
	N	H ^β	H ^{γ2}	Z _{atom}
<i>DMPO-O₂H</i>				
Theoretical	11.87	6.60	1.07	
Experimental (aq) ^b	67%	14.15	11.34	1.58
	33%	14.09	11.78	0.17
Experimental (DMSO) ^c	57%	12.78	10.13	1.39
	43%	12.94	11.66	2.14
<i>AMPO-O₂H</i>				
Theoretical (cis)	12.52	14.53	0.30	
(trans)	11.21	6.68	0.87	
Experimental (aq) ^d	80%	13.0	10.8	
	20%	13.1	12.5	1.75
Experimental (DMSO) ^c	89%	11.15	8.30	0.62
	11%	12.61	9.95	1.56
<i>EMPO-O₂H</i>				
Theoretical (cis)	11.26	14.25	0.30	
(trans)	10.81	8.95	0.68	
Experimental (aq) ^e	54%	12.8	12.1	0.15
	46%	12.8	8.6	
Experimental (DMSO) ^c	59%	12.23	7.71	
	41%	12.31	10.52	
<i>DEPMPO-O₂H</i>				
Theoretical (cis)	10.76	13.51	0.08	P (50.77)
(trans)	11.71	6.60	1.02	P (44.18)
Experimental (aq) ^f	50%	13.2	11.9	52.5
	50%	13.4	10.3	48.5
Experimental(DMSO) ^c	49%	12.30	10.33	48.56
	51%	13.40	11.01	47.16

^a Calculated values are solvent-independent while experimental values were measured from aqueous phase. ^bClement, J.-L., et al., *J. Org. Chem.* **2005**, *70*, 1198-1203.

^cThis work. ^dVillamena, F. A., et al. *J. Org. Chem.* **2004**, *69*, 7994-8004. ^eZhang, H., et al. *FEBS Letters*, **2000**, *473*, 58-62. ^fFrejaville, C., et al. *J. Chem. Soc., Chem. Commun.* **1994**, *15*, 1793-4.

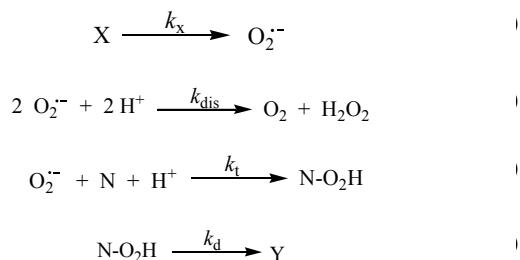
C. Determination of rate constant for AMPO at pH 7.2 using EPR method as described by Tuccio, et al.¹

Experimental:

[AMPO] : 10-200 mM
 [3-carboxy-proxyl] : 0.806 µM
 [xanthine] : 0.8 mM
 [DTPA] : 1 mM
 [xanthine oxidase] : 0.08 u.mL⁻¹
 phosphate buffer 0.1M, pH 7.2

EPR assays were carried out at 20°C in capillary tubes by using a Bruker EMX spectrometer (X band). EPR instrument settings were as follows : modulation frequency, 100 kHz ; modulation amplitude, 1.5 G ; conversion time, 20.48 ms ; time constant, 20.48 ms ; microwave power, 20 mW ; sweep width, 65 G ; sweep time, 10.5 s ; 2 scans. An EPR spectrum was recorded every 21 s for at least 20 min. Kinetics curves were obtained after deconvolution of the signal using the pseudo-inverse method.

Determination of kinetic parameters :



The following model was considered :

in which k_X , k_{dis} , k_T and k_D are the rate constants for the first-order production of superoxide, for the spontaneous dismutation of superoxide, for the superoxide trapping, and for the spin adduct decay, respectively, Y representing EPR silent products and X an intermediate derived from

$$\begin{aligned}
 d[X]/dt &= -k_x [X] \\
 d[O_2^\bullet]/dt &= k_x [X] - k_t [N] [O_2^\bullet] - 2 k_{dis} [O_2^\bullet]^2 \\
 d[N-O_2H]/dt &= k_t [N] [O_2^\bullet] - k_d [N-O_2H] \\
 d[N]/dt &= -k_t [N] [O_2^\bullet]
 \end{aligned}$$

xanthine. The rate eqns. (5)-(8) can be written from this model :

Computer modelling of the kinetic curves was achieved using a the home-made program KALIDAPHNIS and according to eqns. (5)-(8).

Results :

Second order rate constant for the superoxide trapping :

$$k_T = 25.2 \text{ M}^{-1} \text{ s}^{-1} (+/- 1 \text{ M}^{-1} \text{ s}^{-1})$$

First order rate constant for the superoxide adduct decay :

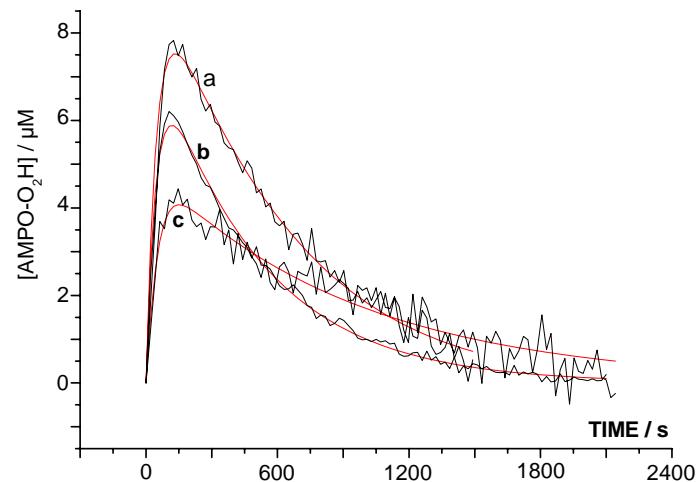
$$[\text{AMPO}] = 200 \text{ mM} \quad k_D = 2.1 \cdot 10^{-3} \text{ s}^{-1} (+/- 0.1 \text{ s}^{-1})$$

$$[\text{AMPO}] = 40 \text{ mM} \quad k_D = 1.7 \cdot 10^{-3} \text{ s}^{-1} (+/- 0.1 \text{ s}^{-1})$$

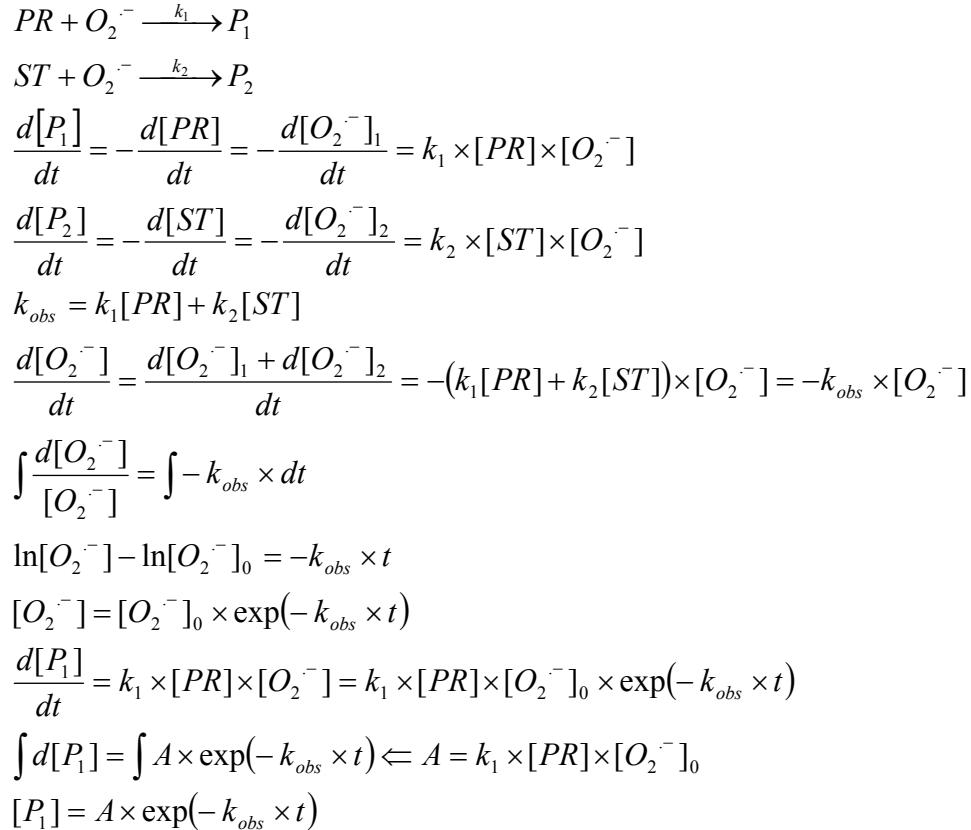
$$[\text{AMPO}] = 10 \text{ mM} \quad k_D = 1.1 \cdot 10^{-3} \text{ s}^{-1} (+/- 0.1 \text{ s}^{-1})$$

Experimental (black) and calculated (red) kinetic curves :

a) [AMPO] = 200 mM, b) [AMPO] = 40 mM, c) [AMPO] = 10 mM.



D. Derivation of Equation 3



where PR = phenol red; SP = spin trap; P₁ is the product which has maximal absorption at 575 nm in 5%H₂O DMF solution. The possibility that the presence of equilibrium concentration of HO₂[•] (pK_a = 4.8¹⁸ or 4.4¹⁹) in water can be attenuated by the sulfonic acid of phenol red is less likely to occur due to the pK_a of phenol red of 7.9²⁰ and that independently measured pH of the final DMF-H₂O solution was found to be ~11. Similarly, protonation of the carbonyl-O in AMPO and EMPO is less likely to occur with pK_{BH+} for esters²¹ and amides²² to be ~−4 and −1, respectively, and is extremely unlikely considering the basic pH of these experiments.

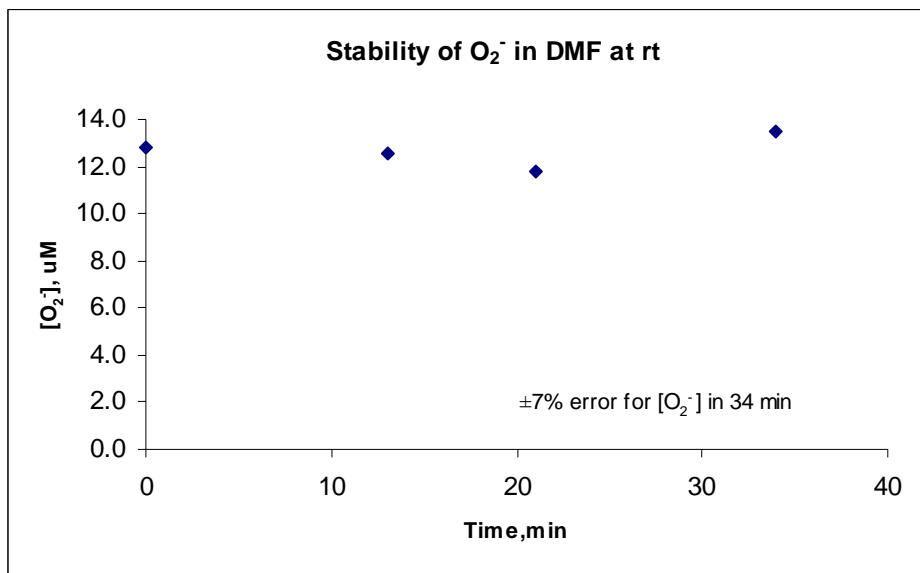


Figure S2. Stability of superoxide in DMF by spectrophotometrically measuring the absorption at 575 nm ($\epsilon = 75,000 \text{ M}^{-1} \text{ cm}^{-1}$) of the species formed upon superoxide reaction with phenol red.

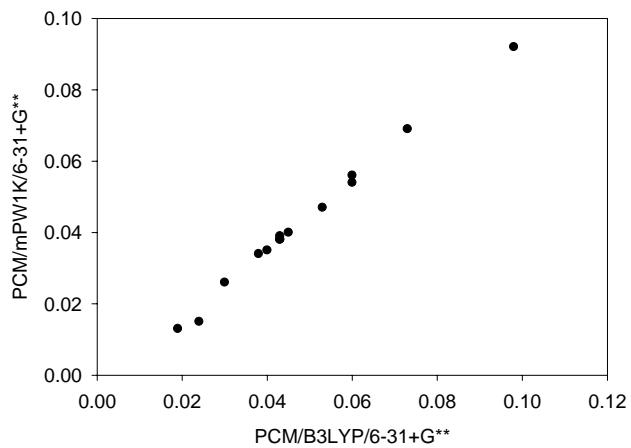
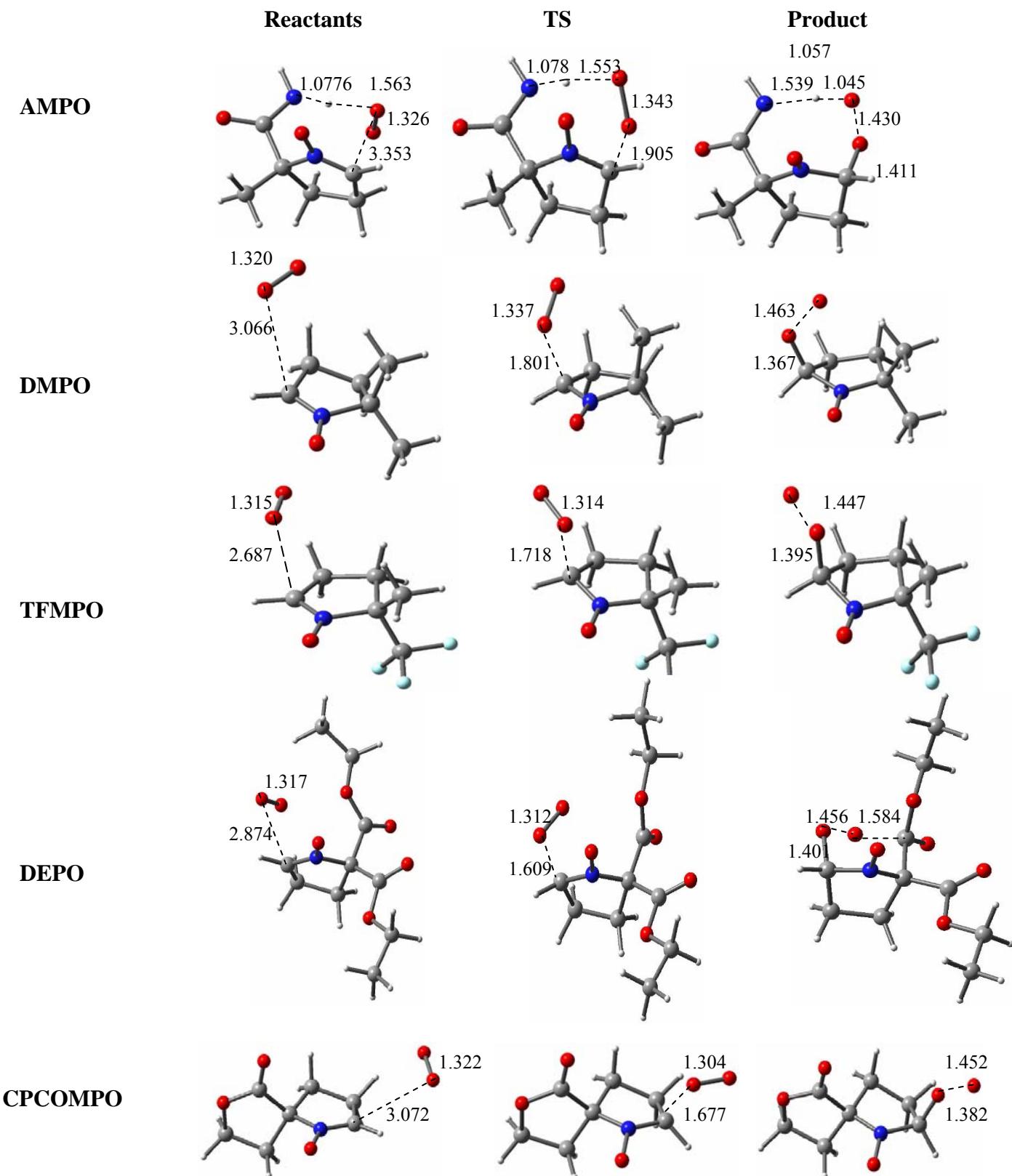
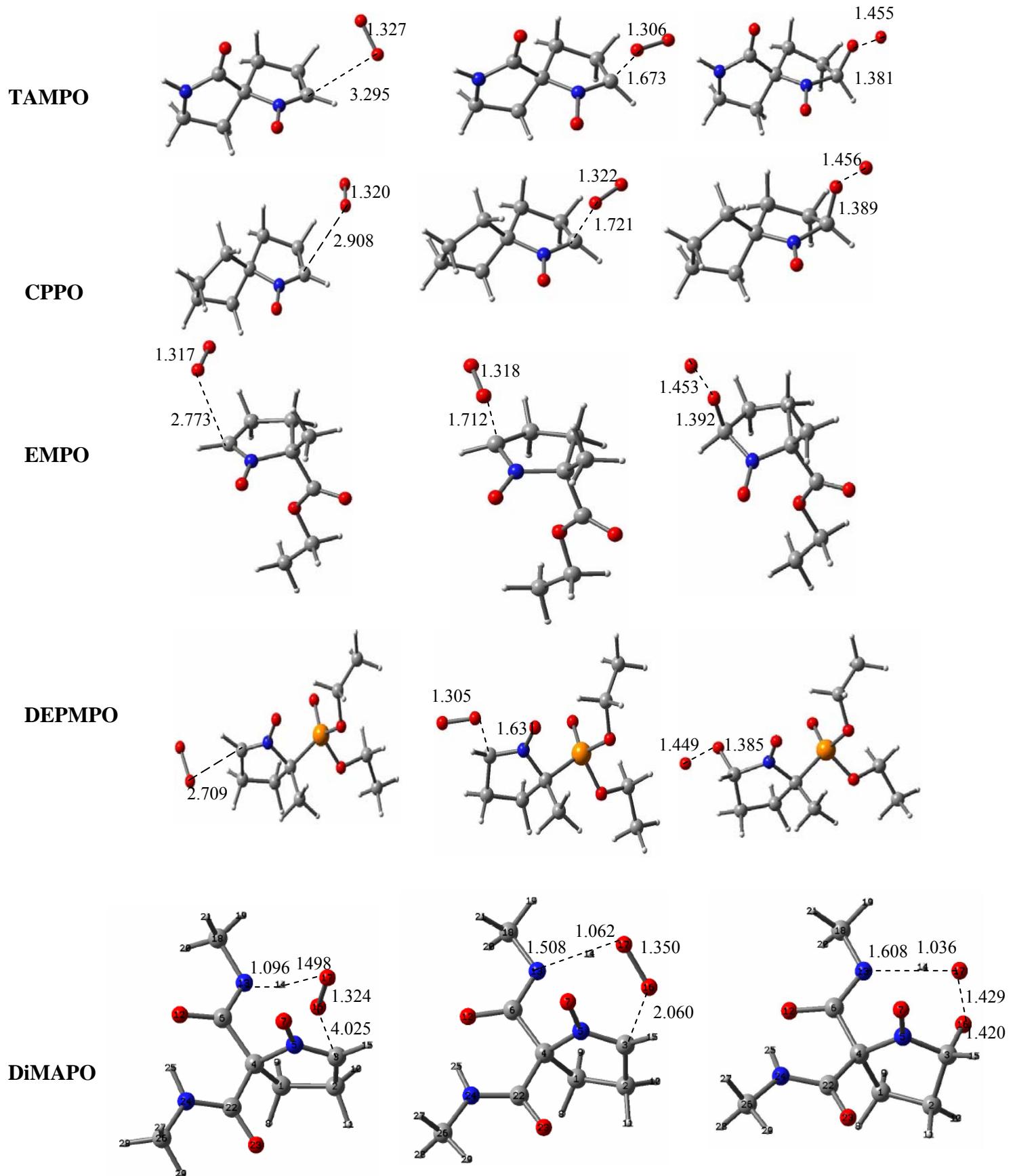
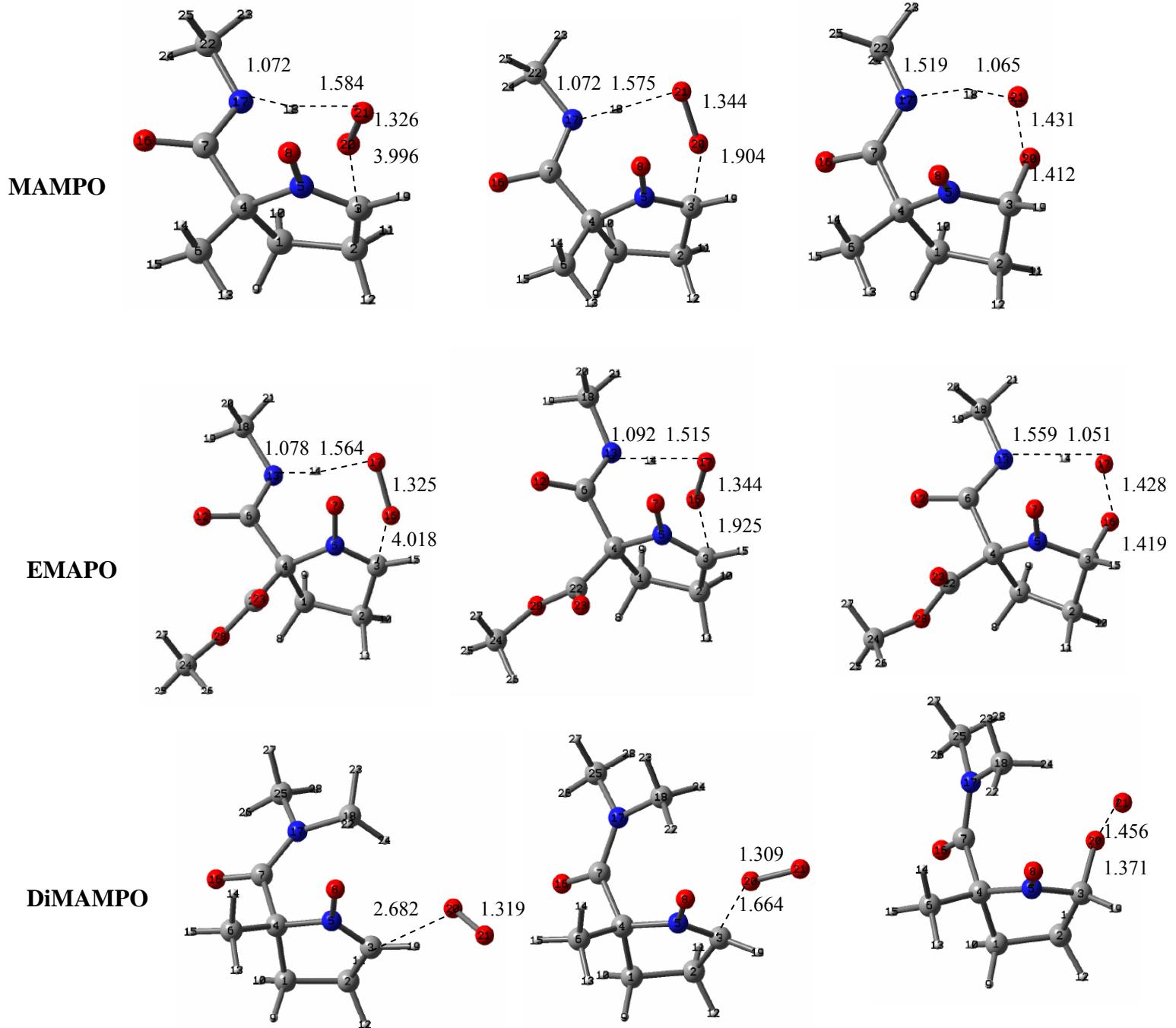


Figure S3. Correlation of the nitronyl-C (C-2) charge densities for various nitrones using PCM(water)/B3LYP/6-31+G(d,p) *versus* PCM(water)/mPW1K/6-31+G(d,p) levels of theory at 298 K ($r^2 = 0.996$).

Figure S4. Optimized Structures at the mPW1K/6-31+G** level of theory.







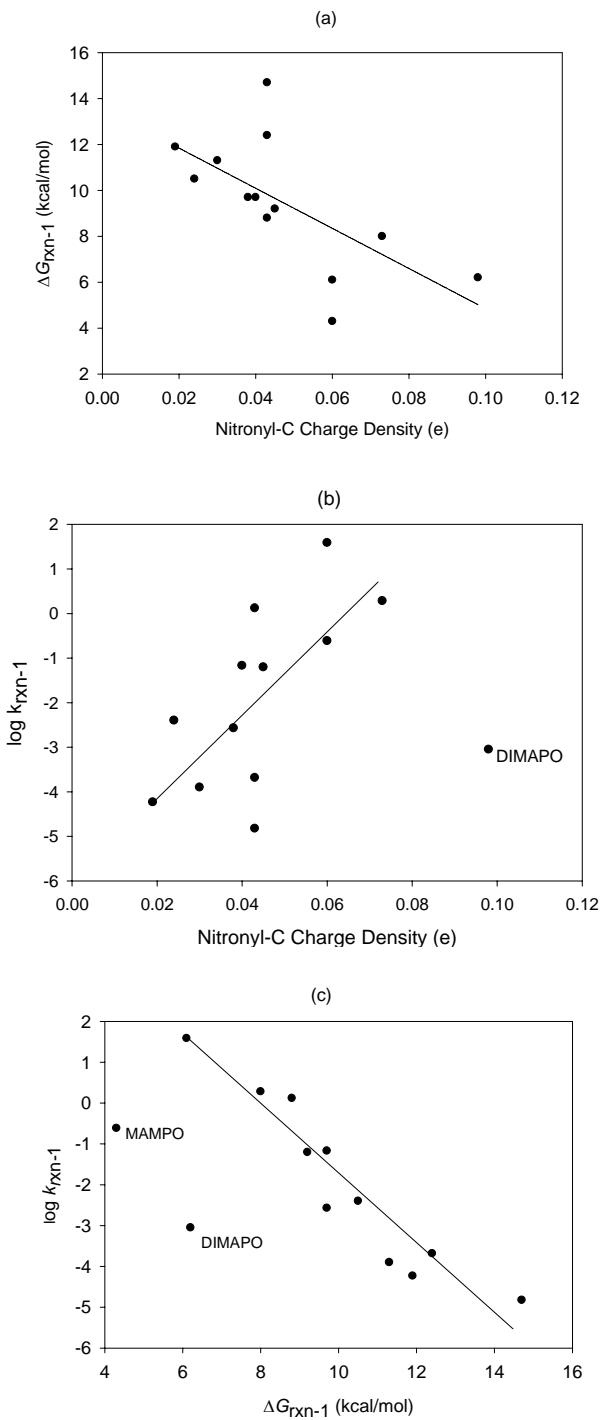


Figure S5. Correlation of the nitronyl-C (C-2) charge densities with that of the (a) free energies ($\Delta G_{\text{rxn-1}}$, 298K, kcal/mol) ($r^2 = 0.42$); and (b) rate constants ($\log k_{\text{rxn-1}}$) of O_2^\cdot addition to nitrones in aqueous phase at the PCM/B3LYP/6-31+G**//B3LYP/6-31G* level of theory at 298 K with $r^2 = 0.48$ excluding the outliers DiMAPO; (c) shows the degree of correlation between $\log k_{\text{rxn-1}}$ and ΔG_{rxn} at the same level of theory with $r^2 = 0.89$, excluding the outliers DiMAPO and MAMPO.

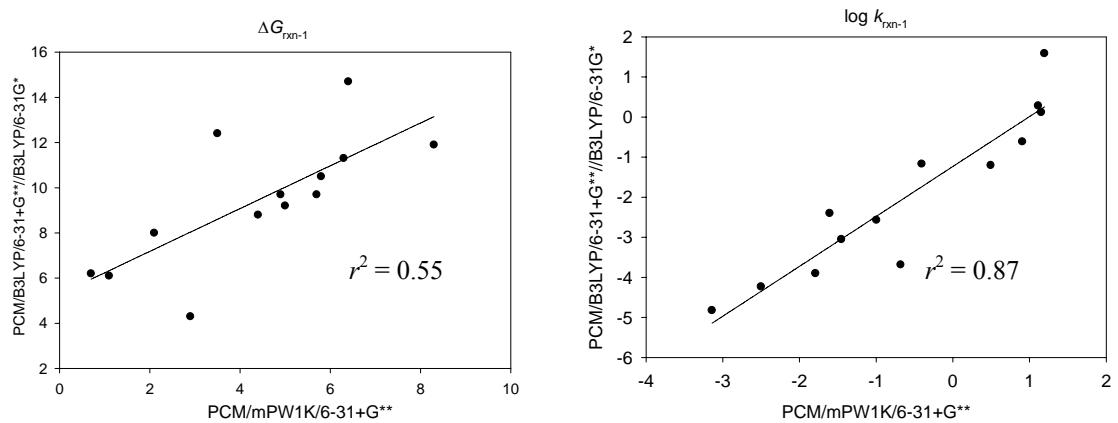


Figure S6. Correlation between the PCM/B3LYP/6-31+G**//B3LYP/6-31G* and mPW1K/6-31+G** for the ΔG_{rxn} and $\log k_{rxn-1}$ of O_2^- addition to nitrones in aqueous phase at 298 K.

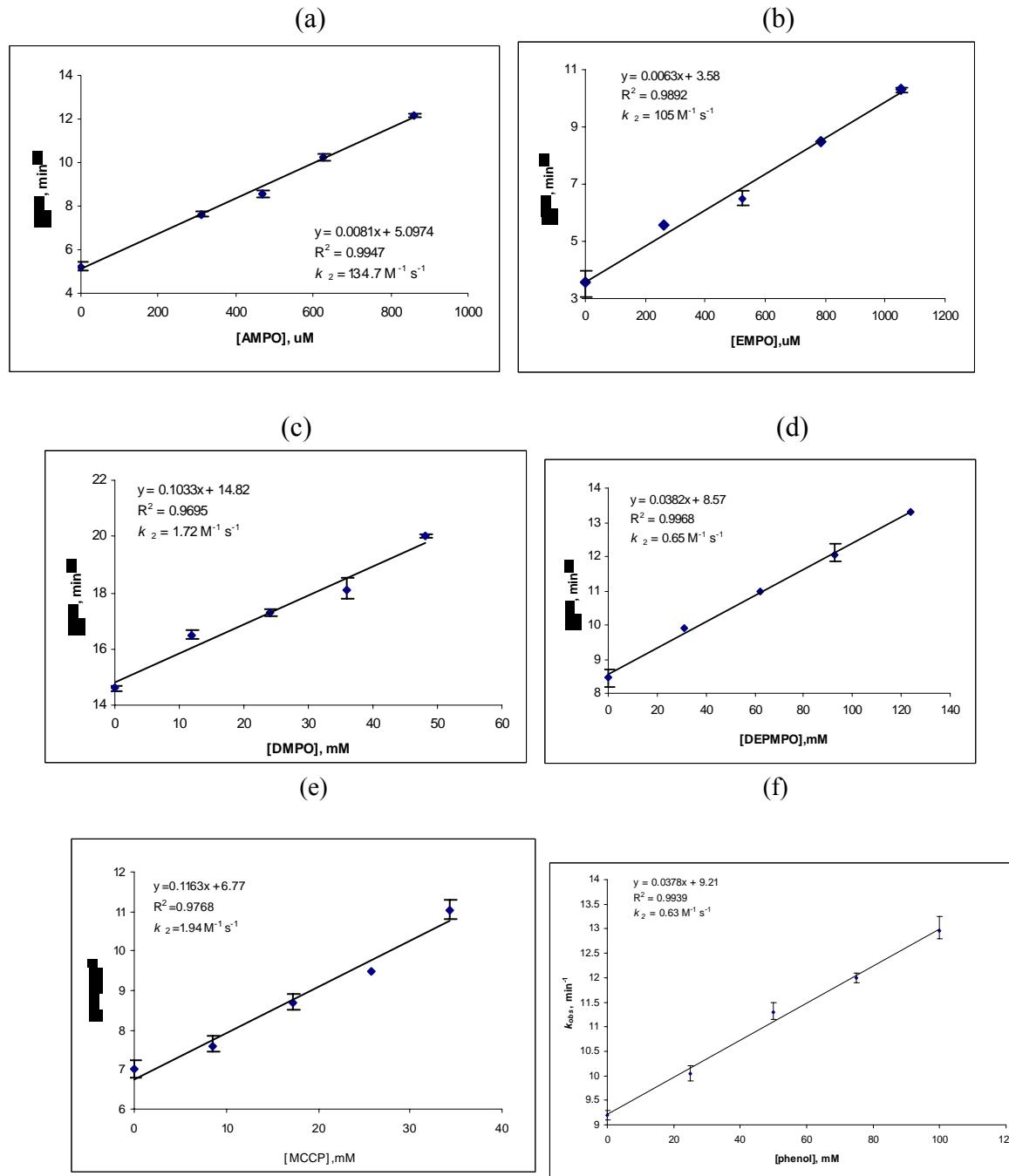


Figure S7. Linear plots of k_{obs} (min⁻¹) for the reaction of superoxide radical anion with various concentrations of (a) AMPO; (b) EMPO; (c) DMPO; (d) DEPMPO; (e) MCCP; and (f) phenol at constant phenol red concentration.

Table S3. Transition State NBO Charges and Spin Densities (Population) of Various Superoxide Adducts at the B3LYP/6-31+G**//B3LYP-6-31G* level.

NBO Charges and Spin Densities ($\alpha-\beta$)				
	N	O _{nitroxyl}	β -O	γ -O
		$\text{O}_2^{\cdot-}$		
AMPO	-0.04, 0.27	-0.49, 0.39	-0.36, 0.24	-0.51, 0.23
DEPMPO	-0.17, 0.04	-0.73, 0.07	-0.22, 0.36	-0.33, 0.55
DMPO	-0.06, 0.22	-0.62, 0.22	-0.32, 0.30	-0.46, 0.36
EMPO	-0.12, 0.01	-0.73, 0.02	-0.26, 0.43	-0.34, 0.57
CPCOMPO	-0.13, 0.06	-0.71, 0.08	-0.24, 0.36	-0.35, 0.53
TAMPO	-0.13, 0.07	-0.71, 0.09	-0.24, 0.36	-0.36, 0.52
TFMPO	-0.12, 0.03	-0.71, 0.05	-0.26, 0.41	-0.35, 0.55
DEPO	-0.08, 0.13	-0.64, 0.14	-0.29, 0.35	-0.40, 0.45
CPPO	-0.10, 0.14	-0.67, 0.15	-0.29, 0.32	-0.42, 0.45
MAMPO	0.01, 0.19	-0.57, 0.21	-0.34, 0.42	-0.48, 0.35
DiMAMPO	-0.15, 0.07	-0.70, 0.07	-0.26, 0.35	-0.33, 0.55
DiMAPO	0.04, 0.17	-0.47, 0.33	-0.31, 0.48	-0.46, 0.19
EMAPO	-0.02, 0.19	-0.51, 0.30	-0.37, 0.33	-0.45, 0.35

Table S3 shows the calculated spin densities for the TS structures for the $\text{O}_2^{\cdot-}$ addition reactions. The spin densities (populations) on the nitronyl-N and nitronyl-O of the TS structures range from 0.01–0.27 e (average: 0.12 ± 0.08 e) and 0.02–0.39 e (average: 0.16 ± 0.12 e), respectively, with the $\text{O}_2^{\cdot-}$ addition of DEPMPO, EMPO, CPCOMPO, TAMPO, TFMPO and DiMAMPO having the lowest spin densities on the nitronyl-N and -O (< 0.1 e) compared to the rest of the $\text{O}_2^{\cdot-}$ adducts. Spin densities on the superoxide-O's are significant with average values of 0.36 ± 0.06 e and 0.43 ± 0.13 e for the β -O and γ -O, respectively. The calculated spin density in $\text{O}_2^{\cdot-}$ itself of 0.5 e for each of the O atoms is much greater than found in the TSs for radical addition, and thereby indicate that a significant amount of electron transfer occurs from the reacting radical to the nitrone unit in the transition states. The electron-transfer characteristics of radical-addition reactions were noted earlier.²³

Table S4. Calculated relative enthalpies ΔH (kcal/mol) and free energies ΔG (kcal/mol) for the formation of various $O_2^{\cdot-}$ adducts at the PCM/mPW1K/6-311+G(3df,2p)//mPW1K/6-31+G(d,p) and PCM/B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d) (in parentheses) levels of theory at 298 K.

Spin Trap (ST)	Enthalpies and Free Energies ^a					
	ST--- $O_2^{\cdot-}$ ^b		[ST + $O_2^{\cdot-}$] ^{‡c}		ST- $O_2^{\cdot-}$ ^d	
	ΔH_{cplx}	ΔG_{cplx}	ΔH^{\ddagger}	ΔG^{\ddagger}	ΔH_{rxn}	ΔG_{rxn}
AMPO	-1.0 (1.3)	7.7 (10.0)	8.5 (9.2)	19.8 (20.9)	-8.7 (-2.5)	2.9 (9.1)
EMPO	2.7 (4.4)	10.4 (13.1)	11.6 (13.4)	21.6 (23.1)	-3.3 (1.9)	6.8 (12.3)
	3.6 (5.8)	11.0 (14.6)	16.0 (17.8)	25.9 (28.6)	0.2 (3.7)	10.9 (14.6)
DEPMPO	4.3 (8.5)	12.8 (18.3)	15.1 (18.2)	26.7 (29.6)	-1.4 (7.4)	9.5 (18.6)

^aEnthalpy, ΔH and Free Energy, ΔG values are all relative to the total ΔH and ΔG values of the ST and $O_2^{\cdot-}$ at infinite separation. ^bST— $O_2^{\cdot-}$ complex. ^cTransition state. ^dProducts.

Table S5. Thermodynamic parameters at the PCM/mPW1K/6-311+g(3df,2p)//mPW1K /6-31+g level of theory.**

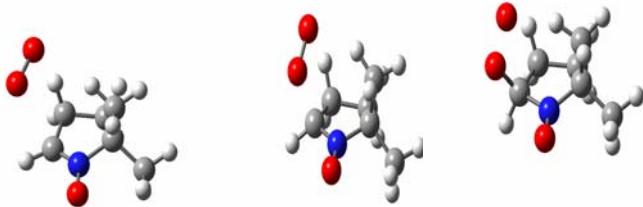
ZPE scaling factor =	hartree to kcal/mol	=
0.9515000		627.5095000



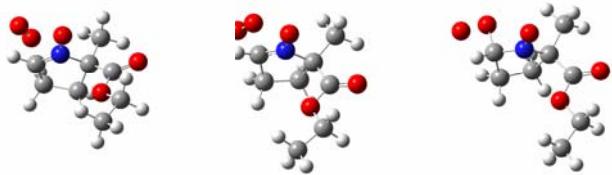
Compound	AMPO-O2 neg	AMPO-O2 TS	AMPO-O2 pos
file	ampO2mpknegF.log	ampO2TSmw.log	ampO2mpk-pos.log
E 6-311+g(3df,2p)	-645.1148071	-645.0976408	-645.1274412
E 6-31+g**	-644.8315807	-644.8120131	-644.8475503
ZPE (raw)	0.1698190	0.1690280	0.1718010
Therm Corr to H (raw)	0.1834590	0.1814570	0.1838630
Therm Corr to G (raw)	0.1293740	0.1314410	0.1345190
H (raw)			
G (raw)			
ZPE (scaled)	0.1615828	0.1608301	0.1634687
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7562000	0.8058000	0.7551000
Symmetry	C1	-	C1
N Imag	0.0000000	1 (511.2355i)	0.0000000
Rotational Con. (GHz)	1.1844700	1.2751343	1.2874600
Rotational Con. (GHz)	0.8101700	0.9132690	0.9337000
Rotational Con. (GHz)	0.6559000	0.7635230	0.7999400
H298			
6-311+g(3df,2p)	-644.9395843	-644.9243817	-644.9519105
6-31+g** tight	-644.6563580	-644.6387540	-644.6720196
G298			
6-311+g(3df,2p)	-644.9936693	-644.9743977	-645.0012545
6-31+g** tight	-644.7104430	-644.6887700	-644.7213636
E	-1.0594237	9.7125964	-8.9874013
H	-1.0060869	8.5337326	-8.7408713
G	7.6585643	19.7517199	2.8988024



Compound	DEPMPO-O2 neg	DEPMPO-O2 TS	DEPMPO-O2 pos
file	depO2mpk-neg.log	depO2TSmw_4F.log	depO2mpk-pos.log
E 6-311+g(3df,2p)	-1201.4115621	-1201.3926557	-1201.4206977
E 6-31+g**	-1201.0063426	-1200.9982674	-1201.0052973
ZPE (raw)	0.2816600	0.2813740	0.2829800
Therm Corr to H (raw)	0.3036690	0.3019460	0.3038040
Therm Corr to G (raw)	0.2282060	0.2313740	0.2321170
H (raw)			
G (raw)			
ZPE (scaled)	0.2679995	0.2677274	0.2692555
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7609000	0.7559000	0.7579000
Symmetry	C1	C1	C1
N Imag	0.0000000	1 (199.2507i)	0.0000000
Rotational Con. (GHz)	0.6829200	0.5963000	0.6243700
Rotational Con. (GHz)	0.2456200	0.3080500	0.3026300
Rotational Con. (GHz)	0.2039400	0.2556900	0.2516100
H298			
6-311+g(3df,2p)	-1201.1215536	-1201.1043563	-1201.1306182
6-31+g** tight	-1200.7163341	-1200.7099680	-1200.7152178
G298			
6-311+g(3df,2p)	-1201.1970166	-1201.1749283	-1201.2023052
6-31+g** tight	-1200.7917971	-1200.7805400	-1200.7869048
E	4.0399953	15.9039221	-1.6926931
H	4.3150427	15.1064748	-1.3731050
G	12.8177964	26.6783775	9.4991246



Compound	DMPO-OO C-O neg	DMPO-OO TS	DMPO-OO C-O pos
file	dmpO2mpk-neg.log	dmpoTSmw_2.log	dmpO2mpk-pos.log
E 6-31+g(3df,2p)	-515.6922488	-515.6706898	-515.6984239
E 6-31+g**	-515.4485250	-515.4292450	-515.4518474
ZPE (raw)	0.1702610	0.1694750	0.1724070
Therm Corr to H (raw)	0.1827760	0.1808050	0.1834960
Therm Corr to G (raw)	0.1307780	0.1329600	0.1368900
H (raw)			
G (raw)			
ZPE (scaled)	0.1620033	0.1612555	0.1640453
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7599000	0.7846000	0.7552000
Symmetry	C1	-	C1
N Imag	0.0000000	- (611.4438i)	0.0000000
Rotational Con. (GHz)	1.9986200	1.9781928	1.9484500
Rotational Con. (GHz)	0.8461800	1.1196951	1.2160000
Rotational Con. (GHz)	0.7871700	1.0242967	1.1282900
H298			
6-311+g(3df,2p)	-515.5177305	-515.4981043	-515.5232896
6-31+g** tight	-515.2740067	-515.2566595	-515.2767131
G298			
6-311+g(3df,2p)	-515.5697285	-515.5459493	-515.5698956
6-31+g** tight	-515.3260047	-515.3045045	-515.3233191
E	3.3499162	16.8784299	-0.5249638
H	3.6466962	15.9623099	0.1583112
G	11.0011075	25.9227682	10.8962538



Compound	EMPO-O2 pos	EMPO-O2 TS	EMPO-O2 neg
file	empO2mpk-pos.log	empoO2TSmw.log	empO2mpk-neg.log
E 6-31+g(3df,2p)	-743.5926549	-743.5766135	-743.6026741
E 6-31+g**	-743.2768394	-743.2651387	-743.2800025
ZPE (raw)	0.2140660	0.2131890	0.2156020
Therm Corr to H (raw)	0.2309350	0.2289480	0.2313100
Therm Corr to G (raw)	0.1676940	0.1694160	0.1720580
H (raw)			
G (raw)			
ZPE (scaled)	0.2036838	0.2028493	0.2051453
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7615000	0.7620000	0.7571000
Symmetry	C1	-	C1
N Imag	0.0000000	1 (586.4555i)	0.0000000
Rotational Con. (GHz)	1.0829000	1.1146011	1.1435200
Rotational Con. (GHz)	0.3943100	0.4572884	0.4614400
Rotational Con. (GHz)	0.3551500	0.4008599	0.4072100
H298			
6-311+g(3df,2p)	-743.3721021	-743.3580051	-743.3818208
6-31+g** tight	-743.0562866	-743.0465304	-743.0591492
G298			
6-311+g(3df,2p)	-743.4353431	-743.4175371	-743.4410728
6-31+g** tight	-743.1195276	-743.1060624	-743.1184012
E	2.3761890	12.4423355	-3.9109686
H	2.7346503	11.5806263	-3.3639382
G	10.4291718	21.6025806	6.8337187

Compound	AMPO	DEPMPO-3	DMPO
file	conh2_mpk_n.log	dep-3_mpk_n.log	dmpo1_mpk_n.log
E 6-311+g(3df,2p)	-494.6436501	-1050.9485314	-365.2281185
E 6-31+g**	-494.4878752	-1050.6760734	-365.1206901
ZPE (raw)	0.1668330	0.2784950	0.1672740
Therm Corr to H (raw)	0.1772260	0.2970740	0.1761550
Therm Corr to G (raw)	0.1324260	0.2311540	0.1355300
H (raw)			
G (raw)			
ZPE (scaled)	0.1587416	0.2649880	0.1591612
Electronic State	1-A	1-A	1-A
s2 6-31g*	0.0000000	0.0000000	0.0000000
Symmetry	C1	C1	C1
N Imag	0.0000000	0.0000000	0.0000000
Rotational Con. (GHz)	1.7698100	0.6582100	2.6357800
Rotational Con. (GHz)	1.3896500	0.4873100	2.2772300
Rotational Con. (GHz)	1.1283800	0.3360000	1.6874200
H298			
6-311+g(3df,2p)	-494.4745155	-1050.6649644	-365.0600763
6-31+g** tight	-494.3187406	-1050.3925064	-364.9526479
G298			
6-311+g(3df,2p)	-494.5193155	-1050.7308844	-365.1007013
6-31+g** tight	-494.3635406	-1050.4584264	-364.9932729

file	Superoxide Radical	EMPO-1
E 6-311+g(3df,2p)	superoxideradical_mw.log	empocis_mpk_n.log
E 6-31+g**	-150.4694688	-593.1269728
ZPE (raw)	-150.3006033	-592.9445344
Therm Corr to H (raw)	0.0028210	0.2109820
Therm Corr to G (raw)	0.0061400	0.2242110
H (raw)	-0.0169530	0.1718010
G (raw)		
ZPE (scaled)		
Electronic State	0.0026842	0.2007494
s2 6-31g*	—	1-A
Symmetry	0.7564000	0.0000000
N Imag	D*H	C1
Rotational Con. (GHz)	0.0000000	0.0000000
Rotational Con. (GHz)	0.0000000	1.3976400
Rotational Con. (GHz)	35.5584482	0.7359900
H298	35.5584482	0.6676100
6-311+g(3df,2p)		
6-31+g** tight	-150.4634656	-592.9129945
G298	-150.2946001	-592.7305561
6-311+g(3df,2p)		
6-31+g** tight	-150.4865586	-592.9654045
	-150.3176931	-592.7829661

Table S6. Thermodynamic parameters at the PCM/B3LYP/6-311+g(3df,2p)// B3LYP /6-31g* level of theory.

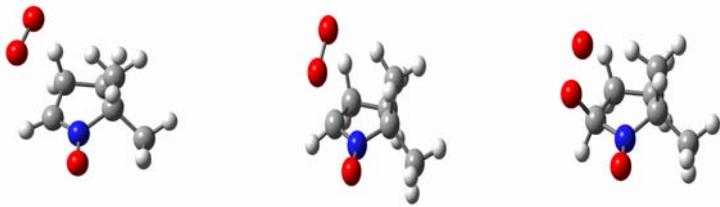
ZPE scaling factor = 0.980600 hartree to kcal/mol = 627.509500



Compound file	AMPO-O2 neg negamp_4.log	AMPO-O2 TS ampTS.log	AMPO-O2 pos posamp.log
E 6-311+g(3df,2p)	-645.285301	-645.270094	-645.291601
E 6-31g*	-644.925901	-644.907357	-644.938433
ZPE (raw)	0.169240	0.167987	0.171001
Therm Corr to H (raw)	0.182815	0.180250	0.183156
Therm Corr to G (raw)	0.128576	0.130692	0.133483
H (raw)			
G (raw)			
ZPE (scaled)	0.165957	0.164728	0.167684
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.755800	0.780000	0.754600
Symmetry	C1	C1	C1
N Imag	0.000000	1 (544.9466i)	0.000000
Rotational Con. (GHz)	1.179271	1.278900	1.282339
Rotational Con. (GHz)	0.795643	0.919840	0.914688
Rotational Con. (GHz)	0.645810	0.765490	0.788613
H298			
6-311+g(3df,2p)	-645.105770	-645.093103	-645.111762
6-31g* tight	-644.746369	-644.730366	-644.758594
G298			
6-311+g(3df,2p)	-645.160009	-645.142661	-645.161435
6-31g* tight	-644.800608	-644.779924	-644.808267
E	1.092830	10.635440	-2.860038
H	1.259771	9.208072	-2.500555
G	9.989683	20.875356	9.094566



Compound	DEPMPO-O2 pos	DEPMPO-O2 TS	DEPMPO-O2 neg
file	posdepo2-TS.log	depO2TScis_newb.log	negdepo2-TS.log
E 6-311+g(3df,2p)	-1201.637929	-1201.620774	-1201.639506
E 6-31g*	-1201.143929	-1201.137452	-1201.141886
ZPE (raw)	0.281245	0.280550	0.281921
Therm Corr to H (raw)	0.302803	0.301171	0.302666
Therm Corr to G (raw)	0.229755	0.230519	0.231743
H (raw)			
G (raw)			
ZPE (scaled)	0.275789	0.275107	0.276452
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.765800	0.754200	0.763100
Symmetry	C1	C1	C1
N Imag	0.000000	1 (391.4737i)	0.000000
Rotational Con. (GHz)	0.557956	0.590050	0.612033
Rotational Con. (GHz)	0.283659	0.306420	0.302179
Rotational Con. (GHz)	0.241784	0.256620	0.250330
H298			
6-311+g(3df,2p)	-1201.340582	-1201.325046	-1201.342309
6-31g* tight	-1200.846583	-1200.841724	-1200.844689
G298			
6-311+g(3df,2p)	-1201.413630	-1201.395698	-1201.413232
6-31g* tight	-1200.919631	-1200.912376	-1200.915612
E	8.256568	19.020935	7.266854
H	8.453150	18.201882	7.369238
G	18.338935	29.591180	18.588480



Compound	DMPO-O2 neg	DMPO-O2 TS	DMPO-O2 pos
file	o2dp_TS-.log	o2dp_292_6311+Gd_1_8_2.log	o2dp_TS+.log
E 6-311+g(3df,2p)	-515.829111	-515.808410	-515.832699
E 6-31g*	-515.520525	-515.503605	-515.520663
ZPE (raw)	0.170068	0.169567	0.171522
Therm Corr to H (raw)	0.182263	0.180654	0.182532
Therm Corr to G (raw)	0.132379	0.133968	0.135986
H (raw)	-515.338262	-515.322950	-515.338130
G (raw)	-515.388146	-515.369636	-515.384676
ZPE (scaled)	0.166769	0.166277	0.168194
Electronic State			
s2 6-31g*	0.760900	0.777500	0.753700
Symmetry	C1	C1	C1
N Imag	0.000000	1.000000	0.000000
Rotational Con. (GHz)	-	-	-
Rotational Con. (GHz)	-	-	-
Rotational Con. (GHz)	-	-	-
H298			
6-311+g(3df,2p)	-515.650148	-515.631046	-515.653495
6-31g* tight	-515.341561	-515.326240	-515.341458
G298	0.000000	13.993318	-0.005880
6-311+g(3df,2p)	-515.700032	-515.677732	-515.700041
6-31g* tight	-515.391445	-515.372926	-515.388004
E	5.502606	18.492712	3.251000
H	5.813899	17.800442	3.713393
G	14.610327	28.603645	14.604448



Compound	EMPO-O2 pos	EMPO-O2 TS	EMPO-O2 neg
file	posemp-o2.log	empoO2TS.log	negemp-o2.log
E 6-311+g(3df,2p)	-743.789610	-743.773640	-743.793635
E 6-31g*	-743.396017	-743.382029	-743.392765
ZPE (raw)	0.213423	0.212576	0.214484
Therm Corr to H (raw)	0.229991	0.228382	0.230151
Therm Corr to G (raw)	0.168589	0.168461	0.171255
H (raw)			
G (raw)			
ZPE (scaled)	0.209283	0.208452	0.210323
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.761300	0.762100	0.758000
Symmetry	C1	C1	C1
N Imag	0.000000	1 (498.0183i)	0.000000
Rotational Con. (GHz)	1.361478	1.163480	1.179920
Rotational Con. (GHz)	0.373926	0.443730	0.448393
Rotational Con. (GHz)	0.355234	0.395970	0.399238
H298			
6-311+g(3df,2p)	-743.563759	-743.549382	-743.567645
6-31g* tight	-743.170166	-743.157771	-743.166775
G298	0.865930	10.817099	0.000000
6-311+g(3df,2p)	-743.625161	-743.609303	-743.626541
6-31g* tight	-743.231568	-743.217692	-743.225671
E	4.137227	14.158406	1.611272
H	4.416290	13.438118	1.977821
G	13.144947	23.096117	12.279017

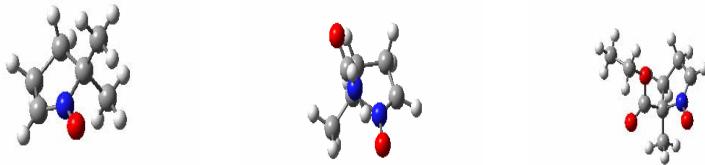
Compound	O2 Radical	AMPO	DMPO
file	o2.log	conh2.log	dmpo1.log
E 6-311+g(3df,2p)	-150.51844	-494.7686029	-365.3194401
E 6-31g*	-150.2996938	-494.5653155	-365.1773173
ZPE (raw)	0.002761	0.166017	0.166744
Therm Corr to H (raw)	0.006082	0.176458	0.175674
Therm Corr to G (raw)	-0.017041	0.13143	0.134895
H (raw)	-150.293612	-494.388857	-365.001643
G (raw)	-150.316735	-494.433885	-365.042422
ZPE (scaled)	0.002707	0.162796	0.163509
Electronic State			
s2 6-31g*	0.7528	0.000000	0.000000
Symmetry	C01	C01	C01
N Imag	0	0.000000	0.000000
Rotational Con. (GHz)	1.63425	1.755748	2.611353
Rotational Con. (GHz)	0.75785	1.375520	2.250094
Rotational Con. (GHz)	0.66048	1.109713	1.6682067
H298			
6-311+g(3df,2p)	-150.512412	-494.595366	-365.147001
6-31g* tight	-150.293665	-494.392078	-365.004878
G298			
6-311+g(3df,2p)	-150.535535	-494.640394	-365.187780
6-31g* tight	-150.316788	-494.437106	-365.045657

Compound	DEPMPO-3	EMPO-1
file	dep-3.log	empocis.log
E 6-311+g(3df,2p)	-1051.132646	-593.2777627
E 6-31g*	-1050.798529	-593.0478221
ZPE (raw)	0.277828	0.210235
Therm Corr to H (raw)	0.296395	0.223456
Therm Corr to G (raw)	0.230716	0.171267
H (raw)	-1050.502134	-592.824366
G (raw)	-1050.567813	-592.876555
ZPE (scaled)	0.272438	0.206156
Electronic State		
s2 6-31g*	0.000000	0.000000
Symmetry	C01	C01
N Imag	0.000000	0.000000
Rotational Con. (GHz)	0.650529	1.397008
Rotational Con. (GHz)	0.483010	0.726683
Rotational Con. (GHz)	0.3335952	0.6549509
H298		
6-311+g(3df,2p)	-1050.841641	-593.058385
6-31g* tight	-1050.507524	-592.828445
G298		
6-311+g(3df,2p)	-1050.907320	-593.110574
6-31g* tight	-1050.573203	-592.880634

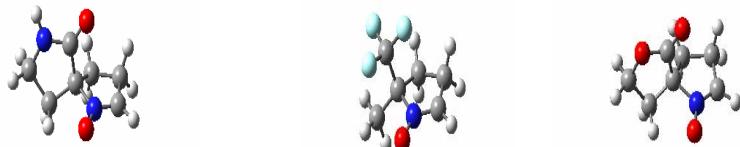
Table S7. Thermodynamic parameters at the PCM/B3LYP/6-31+G//B3LYP/6-31G* level of theory.**

PCM/b3lyp/6-31+g**//b3lyp/6-31g*

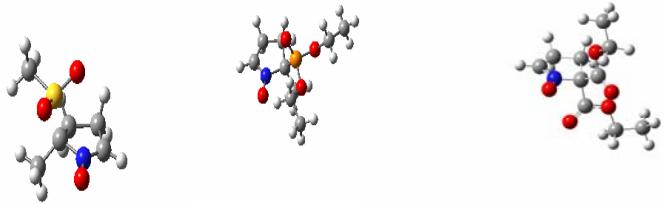
ZPE scaling factor = 0.9806 hartree to kcal/mol = 627.5095



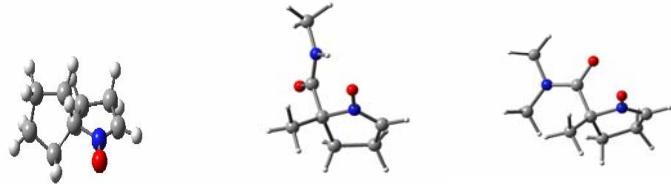
Compound	DMPO file	AMPO	EMPO-1
E 6-31+g** tight PCM	dmpo1.log	-494.613836	-593.088055
E 6-31g*		-494.5653155	-593.0478221
ZPE (raw)	0.166744	0.166017	0.210235
Therm Corr to H (raw)	0.175674	0.176458	0.223456
Therm Corr to G (raw)	0.134895	0.13143	0.171267
H (raw)	-365.001643	-494.388857	-592.824366
G (raw)	-365.042422	-494.433885	-592.876555
ZPE (scaled)	0.163509	0.162796	0.206156
Electronic State			
s2 6-31g*	0.000000	0.000000	0.000000
Symmetry	C01	C01	C01
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	2.611353	1.755748	1.397008
Rotational Con. (GHz)	2.250094	1.375520	0.726683
Rotational Con. (GHz)	1.6682067	1.109713	0.6549509
H298			
6-31+g** tight PCM	-365.035836	-494.440599	-592.868678
6-31g*	-365.004878	-494.392078	-592.828445
G298			
6-31+g** tight PCM	-365.076615	-494.485627	-592.920867
6-31g*	-365.045657	-494.437106	-592.880634



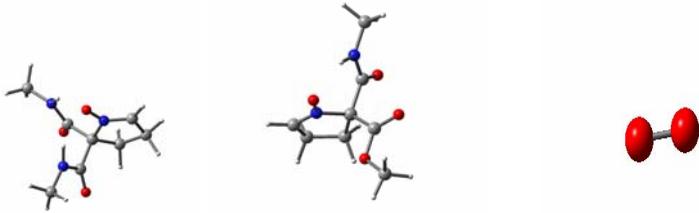
Compound	TAMPO	TFMPO	CPCOMPO
file	lam.log	tfmpo.log	spiro.log
E 6-31+g** tight PCM	-532.716449	-662.941765	-552.567088
E 6-31g*	-532.6611844	-662.8940932	-552.5210662
ZPE (raw)	0.173838	0.143603	0.161224
Therm Corr to H (raw)	0.184087	0.154463	0.171253
Therm Corr to G (raw)	0.139172	0.108489	0.126635
H (raw)	-532.477097	-662.73963	-552.349813
G (raw)	-532.522013	-662.785604	-552.394431
ZPE (scaled)	0.170466	0.140817	0.158096
Electronic State			
s2 6-31g*	0.000000	0.000000	0.000000
Symmetry	C01	C01	C01
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)			1.777462
Rotational Con. (GHz)			1.050776
Rotational Con. (GHz)			0.972269
H298			
6-31+g** tight PCM	-532.535734	-662.790088	-552.398963
6-31g*	-532.480470	-662.742416	-552.352941
G298			
6-31+g** tight PCM	-532.580649	-662.836062	-552.443581
6-31g*	-532.525385	-662.788390	-552.397559



Compound	MSMPO	DEPMPO-3	DEPO Nitrone
file	so2ch3.log	dep-3.log	DEPOb.log
E 6-31+g** tight PCM	-913.786021	-1050.844784	-820.962262
E 6-31g*	-913.7353655	-1050.798529	-820.91136
ZPE (raw)	0.176304	0.277828	0.252889
Therm Corr to H (raw)	0.188712	0.296395	0.270692
Therm Corr to G (raw)	0.139196	0.230716	0.206682
H (raw)	-913.546653	-1050.502134	
G (raw)	-913.596170	-1050.567813	
ZPE (scaled)	0.172884	0.272438	0.247983
Electronic State		1-A	
s2 6-31g*	0.000000	0.000000	0
Symmetry	C0	C01	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.427094	0.650529	0.69608
Rotational Con. (GHz)	0.933019	0.483010	0.40056
Rotational Con. (GHz)	0.838985	0.3335952	0.314700
H298			
6-31+g** tight PCM	-913.600729	-1050.553779	-820.696476
6-31g*	-913.550074	-1050.507524	-820.645574
G298			
6-31+g** tight PCM	-913.650245	-1050.619458	-820.760486
6-31g*	-913.599590	-1050.573203	-820.709584



Compound	CPPO	MAMPO	diMAMPO
file	CPPO.log	mampo.log	diMAMPO_3.log
E 6-31+g** tight PCM	-442.628213	-533.916533	-573.20707
E 6-31g*	-442.5911999	-533.8765506	-573.160583
ZPE (raw)	0.203852	0.194399	0.221908
Therm Corr to H (raw)	0.213742	0.206546	0.235679
Therm Corr to G (raw)	0.169114	0.157121	0.182679
H (raw)	-442.377458		
G (raw)	-442.422085		
ZPE (scaled)	0.199897	0.190628	0.217603
Electronic State			1-A
s2 6-31g*		0	0
Symmetry	C01	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	2.260288	1.6022635	1.508731
Rotational Con. (GHz)	1.154036	0.9445682	0.718530
Rotational Con. (GHz)	0.975120	0.8232683	0.687513
H298			
6-31+g** tight PCM	-442.418426	-533.713758	-572.975696
6-31g*	-442.381413	-533.673776	-572.929209
G298			
6-31+g** tight PCM	-442.463054	-533.763183	-573.028696
6-31g*	-442.426041	-533.723201	-572.982209



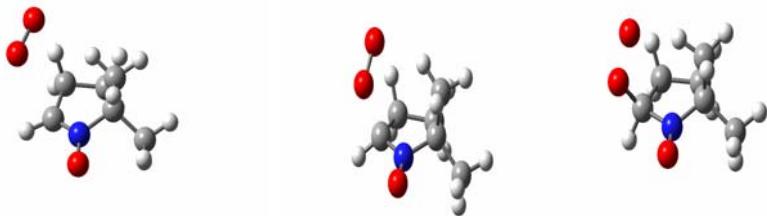
Compound	diMAPO	EMAPO	O2 Radical
file	diAmide_b3lyp_b.log	AMEST_b3lyp.log	o2.log
E 6-31+g** tight PCM	-702.62004	-722.470809	-150.465075
E 6-31g*	-702.569436	-722.4241912	-150.2996938
ZPE (raw)	0.221602	0.208944	0.002761
Therm Corr to H (raw)	0.237143	0.224266	0.006082
Therm Corr to G (raw)	0.17825	0.166673	-0.017041
H (raw)			-150.293612
G (raw)			-150.316735
ZPE (scaled)	0.217303	0.204890	0.002707
Electronic State	1-A	1-A	
s2 6-31g*	0	0	0.7528
Symmetry	C1	C1	C01
N Imag	0.000000	0.000000	0
Rotational Con. (GHz)	0.7483062	0.8696075	1.63425
Rotational Con. (GHz)	0.6732812	0.6410939	0.75785
Rotational Con. (GHz)	0.5456517	0.5181203	0.66048
H298			
6-31+g** tight PCM	-702.387196	-722.250597	-150.459047
6-31g*	-702.336592	-722.203979	-150.293665
G298			
6-31+g** tight PCM	-702.446089	-722.308190	-150.482170
6-31g*	-702.395485	-722.261572	-150.316788



Compound	AMPO-O2 neg	AMPO-O2 TS	AMPO-O2 pos
file	negamp_4.log	ampTS.log	posamp.log
E 6-31+g** tight PCM	-645.079408	-645.067551	-645.088217
E 6-31g*	-644.925901	-644.907357	-644.938433
ZPE (raw)	0.169240	0.167987	0.171001
Therm Corr to H (raw)	0.182815	0.180250	0.183156
Therm Corr to G (raw)	0.128576	0.130692	0.133483
H (raw)			
G (raw)			
ZPE (scaled)	0.165957	0.164728	0.167684
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.755800	0.780000	0.754600
Symmetry	C1	C1	C1
N Imag	0.000000	1 (544.9466i)	0.000000
Rotational Con. (GHz)	1.179271	1.278900	1.282339
Rotational Con. (GHz)	0.795643	0.919840	0.914688
Rotational Con. (GHz)	0.645810	0.765490	0.788613
H298			
6-31+g** tight PCM	-644.899876	-644.890560	-644.908378
6-31g* tight	-644.746369	-644.730366	-644.758594
G298			
6-31+g** tight PCM	-644.954115	-644.940118	-644.958051
6-31g* tight	-644.800608	-644.779924	-644.808267
E	-0.311872	7.128508	-5.839603
H	-0.144931	5.701141	-5.480120
G	8.584981	17.368425	6.115001



Compound	DEPMPO-O2 pos	DEPMPO-O2 TS	DEPMPO-O2 neg
file	posdepo2-TS.log	depO2TScis_newb.log	negdepo2-TS.log
E 6-31+g** tight PCM	-1201.299854	-1201.285189	-1201.304526
E 6-31g*	-1201.143929	-1201.137452	-1201.141886
ZPE (raw)	0.281245	0.280550	0.281921
Therm Corr to H (raw)	0.302803	0.301171	0.302666
Therm Corr to G (raw)	0.229755	0.230519	0.231743
H (raw)			
G (raw)			
ZPE (scaled)	0.275789	0.275107	0.276452
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.765800	0.754200	0.763100
Symmetry	C1	C1	C1
N Imag	0.000000	1 (391.4737i)	0.000000
Rotational Con. (GHz)	0.557956	0.590050	0.612033
Rotational Con. (GHz)	0.283659	0.306420	0.302179
Rotational Con. (GHz)	0.241784	0.256620	0.250330
H298			
6-31+g** tight PCM	-1201.002507	-1200.989461	-1201.007329
6-31g* tight	-1200.846583	-1200.841724	-1200.844689
G298			
6-31+g** tight PCM	-1201.075555	-1201.060113	-1201.078252
6-31g* tight	-1200.919631	-1200.912376	-1200.915612
E	6.278233	15.480659	3.346508
H	6.474815	14.661607	3.448892
G	16.360599	26.050904	14.668134



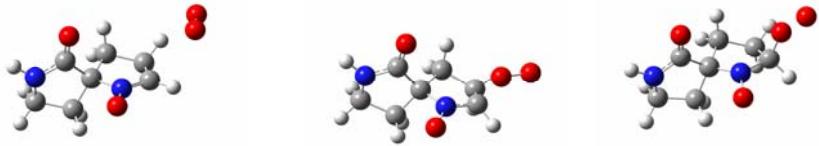
Compound	DMPO-O2 neg	DMPO-O2 TS	DMPO-O2 pos
file	o2dp_TS-.log	o2dp_292_6311+Gd_1_8_2.l og	o2dp_TS+.log
E 6-31+g** tight PCM	-515.665399	-515.648461	-515.672512
E 6-31g*	-515.520525	-515.503605	-515.520663
ZPE (raw)	0.170068	0.169567	0.171522
Therm Corr to H (raw)	0.182263	0.180654	0.182532
Therm Corr to G (raw)	0.132379	0.133968	0.135986
H (raw)	-515.338262	-515.322950	-515.338130
G (raw)	-515.388146	-515.369636	-515.384676
ZPE (scaled)	0.166769	0.166277	0.168194
Electronic State			
s2 6-31g*	0.760900	0.777500	0.753700
Symmetry	C1	C1	C1
N Imag	0.000000	1.000000	0.000000
Rotational Con. (GHz)	-	-	-
Rotational Con. (GHz)	-	-	-
Rotational Con. (GHz)	-	-	-
H298			
6-31+g** tight PCM	-515.486435	-515.471097	-515.493308
6-31g* tight	-515.341561	-515.326240	-515.341458
G298	0.000000	11.631968	-2.217749
6-31+g** tight PCM	-515.536319	-515.517783	-515.539854
6-31g* tight	-515.391445	-515.372926	-515.388004
E	4.989328	15.618084	0.525853
H	5.300622	14.925814	0.988246
G	14.097050	25.729017	11.879301



Compound	EMPO-O2 pos	EMPO-O2 TS	EMPO-O2 neg
file	posemp-o2.log	empoO2TS.log	negemp-o2.log
E 6-31+g** tight PCM	-743.548068	-743.533737	-743.554695
E 6-31g*	-743.396017	-743.382029	-743.392765
ZPE (raw)	0.213423	0.212576	0.214484
Therm Corr to H (raw)	0.229991	0.228382	0.230151
Therm Corr to G (raw)	0.168589	0.168461	0.171255
H (raw)			
G (raw)			
ZPE (scaled)	0.209283	0.208452	0.210323
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.761300	0.762100	0.758000
Symmetry	C1	C1	C1
N Imag	0.000000	1 (498.0183i)	0.000000
Rotational Con. (GHz)	1.361478	1.163480	1.179920
Rotational Con. (GHz)	0.373926	0.443730	0.448393
Rotational Con. (GHz)	0.355234	0.395970	0.399238
H298			
6-31+g** tight PCM	-743.322217	-743.309479	-743.328705
6-31g* tight	-743.170166	-743.157771	-743.166775
G298	2.498481	11.421310	0.000000
6-31+g** tight PCM	-743.383619	-743.369400	-743.387601
6-31g* tight	-743.231568	-743.217692	-743.225671
E	3.176453	12.169292	-0.982052
H	3.455517	11.449004	-0.615503
G	12.184174	21.107002	9.685692



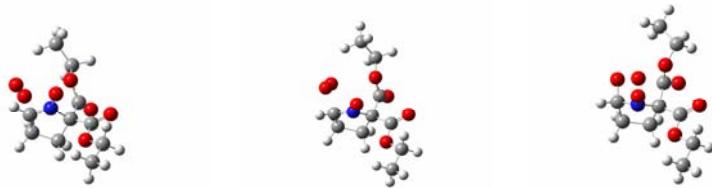
Compound	CPCOMPO-O2 neg	CPCOMPO-O2 TS	CPCOMPO-O2 pos
file	negtonO2_F.log	tonO2TSd.log	postonO2.log
E 6-31+g** tight PCM	-703.025818	-703.013386	-703.034450
E 6-31g*	-702.866580	-702.856912	-702.865836
ZPE (raw)	0.164170	0.163595	0.165153
Therm Corr to H (raw)	0.177558	0.176062	0.177559
Therm Corr to G (raw)	0.123382	0.124525	0.126577
H (raw)			
G (raw)			
ZPE (scaled)	0.160985	0.160421	0.161949
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.770300	0.755400	0.760600
Symmetry	C1	C1	C1
N Imag	0.000000	1 (503.6489i)	0.000000
Rotational Con. (GHz)	1.490370	1.562580	1.606469
Rotational Con. (GHz)	0.480851	0.553570	0.556095
Rotational Con. (GHz)	0.474229	0.535570	0.539044
H298			
6-31+g** tight PCM	-702.851445	-702.840498	-702.860095
6-31g* tight	-702.692207	-702.684023	-702.691481
G298			
6-31+g** tight PCM	-702.905621	-702.892035	-702.911077
6-31g* tight	-702.746383	-702.735560	-702.742463
E	3.981548	11.782746	-1.435114
H	4.119230	10.988674	-1.308771
G	12.631397	21.156838	9.207661



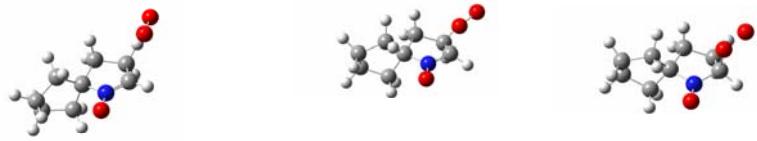
Compound	TAMPO-O2 neg	TAMPO-O2 TS	TAMPO-O2 pos
file	neglam_O2.log	lamO2TSd.log	poslam_O2.log
E 6-31+g** tight PCM	-683.174376	-683.159494	-683.182780
E 6-31g*	-682.999732	-682.988632	-682.998353
ZPE (raw)	0.176512	0.175991	0.177594
Therm Corr to H (raw)	0.190225	0.188723	0.190269
Therm Corr to G (raw)	0.135259	0.136799	0.138839
H (raw)			
G (raw)			
ZPE (scaled)	0.173088	0.172577	0.174149
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.763400	0.755900	0.759500
Symmetry	C1	C1	C1
N Imag	0.000000	1 (528.7335i)	0.000000
Rotational Con. (GHz)	1.502850	1.545800	1.587784
Rotational Con. (GHz)	0.461066	0.552980	0.555984
Rotational Con. (GHz)	0.455804	0.533340	0.538506
H298			
6-31+g** tight PCM	-682.987575	-682.974185	-682.995956
6-31g* tight	-682.812932	-682.803323	-682.811529
G298			
6-31+g** tight PCM	-683.042541	-683.026109	-683.047386
6-31g* tight	-682.867898	-682.855247	-682.862959
E	4.485438	13.824034	-0.788152
H	4.521638	12.924057	-0.737514
G	12.724442	23.035745	9.684164



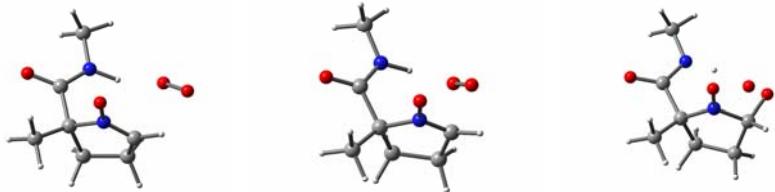
Compound	TFMPO-O2 neg	TFMPO-O2 TS	TFMPO-O2 pos
file	postfO2c.log	tfTS.log	postf.log
E 6-31+g** tight PCM	-813.401644	-813.390593	-813.410330
E 6-31g*	-813.244360	-813.233406	-813.244841
ZPE (raw)	0.146946	0.146385	0.148186
Therm Corr to H (raw)	0.161265	0.159833	0.161406
Therm Corr to G (raw)	0.104893	0.105956	0.108922
H (raw)			
G (raw)			
ZPE (scaled)	0.144095	0.143545	0.145311
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.762400	0.754300	0.758100
Symmetry	C1	C1	C1
N Imag	0.000000	1 (374.3011i)	0.000000
Rotational Con. (GHz)	1.403215	1.505130	1.511714
Rotational Con. (GHz)	0.516346	0.540180	0.573292
Rotational Con. (GHz)	0.485744	0.504960	0.534636
H298			
6-31+g** tight PCM	-813.243230	-813.233600	-813.251799
6-31g* tight	-813.085946	-813.076413	-813.086310
G298			
6-31+g** tight PCM	-813.299602	-813.287477	-813.304283
6-31g* tight	-813.142318	-813.130290	-813.138794
E	3.260539	10.195147	-2.190008
H	3.705261	9.748104	-1.671903
G	11.690320	19.298799	8.752912



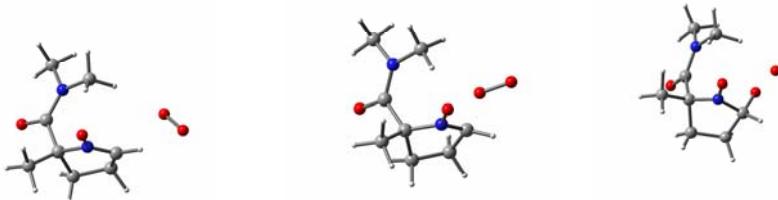
Compound	DEPO-OO pos	DEPO-OO TS TS	DEPO-OO neg
file	posdepoo2.log	DEPO_O2TS.log	negdepoo2.log
E 6-31+g** tight PCM	-971.419874	-971.403402	-971.429743
E 6-31g*	-971.268072	-971.253574	-971.283457
ZPE (raw)	0.256941	0.255761	0.258871
Therm Corr to H (raw)	0.277542	0.275858	0.277716
Therm Corr to G (raw)	0.207553	0.205517	0.211851
H (raw)			
G (raw)			
ZPE (scaled)	0.251956	0.250799	0.253849
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.760000	0.766600	0.754500
Symmetry	C1	C1	C1
N Imag	0.000000	1 (559.0564i)	0.000000
Rotational Con. (GHz)	0.738529	0.694160	0.688850
Rotational Con. (GHz)	0.278483	0.305200	0.339918
Rotational Con. (GHz)	0.249665	0.269340	0.283969
H298			
6-31+g** tight PCM	-971.147317	-971.132506	-971.157049
6-31g* tight	-970.995515	-970.982678	-971.010763
G298			
6-31+g** tight PCM	-971.217306	-971.202847	-971.222914
6-31g* tight	-971.065504	-971.053019	-971.076628
E	4.683103	15.019440	-1.509788
H	5.149314	14.443290	-0.957885
G	15.907337	24.980429	12.387987



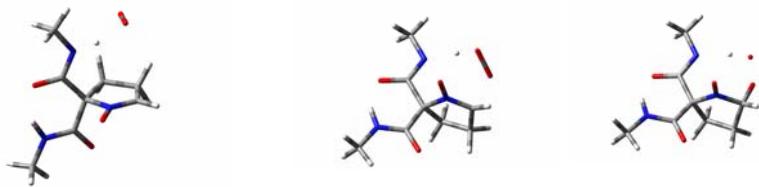
Compound	CPPO-OO neg	CPPO-OO TS	CPPO-OO pos
file	cpp-o2-b3lyp-neg.log	CPPO-OO-b3lypTS2.log	cpp-o2-b3lyp-pos.log
E 6-31+g** PCM	-593.085881	-593.071291	-593.092605
E 6-31g*	-592.933673	-592.919490	-592.929906
ZPE (raw)	0.207113	0.206208	0.208078
Therm Corr to H (raw)	0.220137	0.218395	0.220278
Therm Corr to G (raw)	0.166857	0.167067	0.168147
H (raw)			
G (raw)			
ZPE (scaled)	0.203095	0.202208	0.204041
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.761100	0.760300	0.757800
Symmetry	C1	C1	C1
N Imag	0.000000	1 (542.8066i)	0.000000
Rotational Con. (GHz)	1.842460	1.858990	1.824273
Rotational Con. (GHz)	0.531615	0.612810	0.646861
Rotational Con. (GHz)	0.505726	0.580410	0.615310
H298			
6-31+g** PCM	-592.869762	-592.856896	-592.876364
6-31g*	-592.717554	-592.705095	-592.713664
G298			
6-31+g** PCM	-592.923042	-592.908224	-592.928495
6-31g*	-592.770834	-592.756423	-592.765795
E	4.647963	13.803326	0.428589
H	4.838286	12.911546	0.695644
G	13.918976	23.217134	10.497342



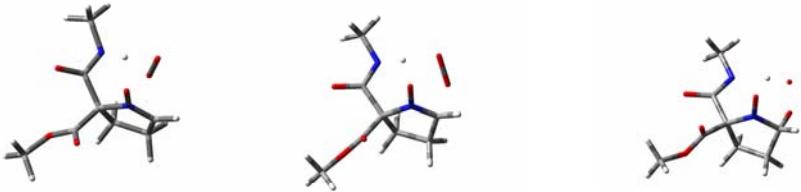
Compound	MAMPO-O2 neg	MAMPO-OO TS	MAMPO-O2 pos
file	MAMPO_OOb3lyp-neg.log	MAMPO_O2-cis1a_TS_b3lyp.log	MAMPO_OOb3lyp-pos.log
E 6-31+g** PCM	-684.380303	-684.365326	-684.392812
E 6-31g*	-684.233328	-684.218003	-684.249834
ZPE (raw)	0.197295	0.196720	0.197750
Therm Corr to H (raw)	0.212603	0.211033	0.211771
Therm Corr to G (raw)	0.155431	0.156114	0.158132
H (raw)			
G (raw)			
ZPE (scaled)	0.193467	0.192904	0.193914
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.756900	0.791300	0.754500
Symmetry	C1	C1	C1
N Imag	0.000000	1 (342.5210i)	0.000000
Rotational Con. (GHz)	0.932179	0.944420	1.043728
Rotational Con. (GHz)	0.740176	0.836850	0.802565
Rotational Con. (GHz)	0.540506	0.603070	0.619112
H298			
6-31+g** PCM	-684.171528	-684.158109	-684.184877
6-31g*	-684.024553	-684.010787	-684.041899
G298			
6-31+g** PCM	-684.228700	-684.213028	-684.238516
6-31g*	-684.081725	-684.065706	-684.095538
E	0.818900	10.217110	-7.030616
H	0.801569	9.221588	-7.575575
G	10.450155	20.283953	4.290003



Compound	diMAMPO-O2 neg	diMAMPO-O2 TS	diMAMPO-O2 pos
file	dimamO2b3lyp-neg.log	diMAMPO_O2-3_TS_b3lyp_c.log	dimamO2b3lyp-pos.log
E 6-31+g** PCM	-723.665990	-723.650854	-723.674151
E 6-31g*	-723.518670	-723.510751	-723.519609
ZPE (raw)	0.226513	0.225661	0.227283
Therm Corr to H (raw)	0.243044	0.241132	0.242882
Therm Corr to G (raw)	0.182975	0.183826	0.185747
H (raw)			
G (raw)			
ZPE (scaled)	0.222119	0.221283	0.222874
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.758900	0.754500	0.756400
Symmetry	C1	C1	C1
N Imag	0.000000	1 (311.4001i)	0.000000
Rotational Con. (GHz)	0.869498	0.842360	0.834055
Rotational Con. (GHz)	0.549226	0.646450	0.724833
Rotational Con. (GHz)	0.448125	0.523760	0.589458
H298			
6-31+g** PCM	-723.427340	-723.414100	-723.435678
6-31g*	-723.280021	-723.273996	-723.281137
G298			
6-31+g** PCM	-723.487409	-723.471406	-723.492813
6-31g*	-723.340090	-723.331302	-723.338272
E	3.862321	13.360305	-1.258784
H	4.644967	12.953525	-0.587168
G	14.719005	24.761371	11.327982



Compound	diMAPO-O2 neg	diMAPO-O2 TS	diMAPO-O2 pos
file	neg-diMAPO_O2b3lyp_e.log	diMAPO_O2_b3lyp_e.log	pos-diMAPO_O2b3lyp_e.log
E 6-31+g** PCM	-853.086696	-853.063836	-853.095649
E 6-31g*	-852.937347	-852.919890	-852.954730
ZPE (raw)	0.224385	0.223330	0.226278
Therm Corr to H (raw)	0.242874	0.240584	0.243367
Therm Corr to G (raw)	0.176639	0.178232	0.181606
H (raw)			
G (raw)			
ZPE (scaled)	0.220032	0.218997	0.221888
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.754200	0.806300	0.753500
Symmetry	-	C1	-
N Imag	0.000000	1 (410.6112i)	0.000000
Rotational Con. (GHz)	0.773198	0.760760	0.760166
Rotational Con. (GHz)	0.418748	0.475550	0.486947
Rotational Con. (GHz)	0.339072	0.353810	0.363148
H298			
6-31+g** PCM	-852.848175	-852.827585	-852.856672
6-31g*	-852.698826	-852.683639	-852.715753
G298			
6-31+g** PCM	-852.914410	-852.889937	-852.918433
6-31g*	-852.765061	-852.745991	-852.777514
E	-0.992093	13.352775	-6.610185
H	-1.212616	11.708097	-6.544391
G	8.690111	24.047444	6.165814



Compound	EMAPO-O2 neg	EMAPO-O2 TS	EMAPO-O2 pos
file	EMAPO_O2b3lypF_pcm.l og	EMAPO_O2_b3lyp_h.lo g	pos- EMAPO_O2b3lyp.log
E 6-31+g** PCM	-872.937149	-872.921721	-872.942361
E 6-31g*	-872.786251	-872.765273	-872.799038
ZPE (raw)	0.211689	0.210558	0.213220
Therm Corr to H (raw)	0.230140	0.227878	0.230237
Therm Corr to G (raw)	0.164547	0.165903	0.168904
H (raw)			
G (raw)			
ZPE (scaled)	0.207582	0.206473	0.209084
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.755500	0.798300	0.753400
Symmetry	C1	C1	-
N Imag	0.000000	1 (471.8182i)	0.000000
Rotational Con. (GHz)	0.713602	0.782580	0.779934
Rotational Con. (GHz)	0.419715	0.463500	0.471274
Rotational Con. (GHz)	0.366952	0.368760	0.376353
H298			
6-31+g** PCM	-872.711116	-872.697928	-872.716260
6-31g*	-872.560218	-872.541480	-872.572937
G298			
6-31+g** PCM	-872.776709	-872.759903	-872.777593
6-31g*	-872.625811	-872.603455	-872.634270
E	-0.793800	8.887417	-4.064379
H	-0.924127	7.351432	-4.152476
G	8.565699	19.111587	8.010541

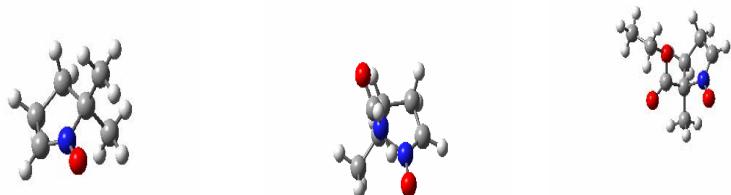
Table S8. Thermodynamic parameters at the PCM/mPW1K/6-31+G level of theory.**

PCM/mpw1K/6-31+g**

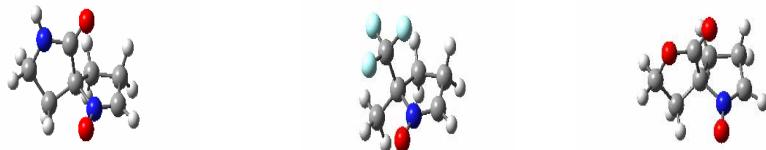
ZPE scaling factor =

0.9515 hartree to kcal/mol =

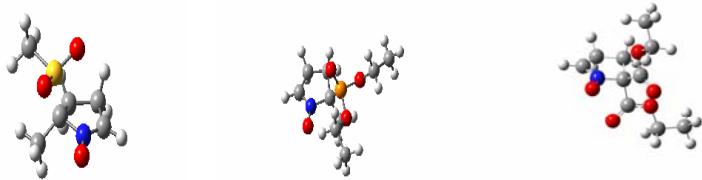
627.5095



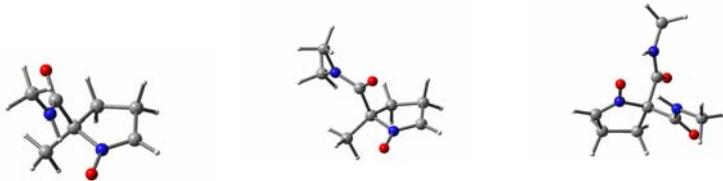
Compound	DMPO	AMPO	EMPO-1
file	dmpo1_mpk_n.log	conh2_mpk_n.log	empocis_mpk_n.log
E 6-31+g** tight PCM	-365.121503	-494.496016	-592.94393
E 6-31+g**	-365.1206901	-494.4878752	-592.9445344
ZPE (raw)	0.167274	0.166833	0.210982
Therm Corr to H (raw)	0.176155	0.177226	0.224211
Therm Corr to G (raw)	0.13553	0.132426	0.171801
H (raw)			
G (raw)			
ZPE (scaled)	0.159161	0.158742	0.200749
Electronic State	1-A	1-A	1-A
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	2.635780	1.769810	1.397640
Rotational Con. (GHz)	2.277230	1.389650	0.735990
Rotational Con. (GHz)	1.687420	1.128380	0.667610
H298			
6-31+g** tight PCM	-364.953461	-494.326881	-592.729952
6-31+g**	-364.952648	-494.318741	-592.730556
G298			
6-31+g** tight PCM	-364.994086	-494.371681	-592.782362
6-31+g**	-364.993273	-494.363541	-592.782966



Compound	TAMPO	TFMPO	CPCOMPO
file	lam_mpk_n.log	tfmpo_mpk_n.log	spiro_mpk_n.log
E 6-31+g** tight PCM	-532.594724	-662.788986	-552.438301
E 6-31+g**	-532.5780632	-662.7867733	-552.4271754
ZPE (raw)	0.174956	0.144077	0.162231
Therm Corr to H (raw)	0.185131	0.154941	0.172189
Therm Corr to G (raw)	0.140397	0.108892	0.12773
H (raw)			
G (raw)			
ZPE (scaled)	0.166471	0.137089	0.154363
Electronic State	1-A	1-A	1-A
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.771360	1.555030	1.791900
Rotational Con. (GHz)	1.058880	1.100720	1.058800
Rotational Con. (GHz)	0.976090	0.973780	0.984670
H298			
6-31+g** tight PCM	-532.418078	-662.641033	-552.273980
6-31+g**	-532.401418	-662.638820	-552.262855
G298			
6-31+g** tight PCM	-532.462812	-662.687082	-552.318439
6-31+g**	-532.446152	-662.684869	-552.307314



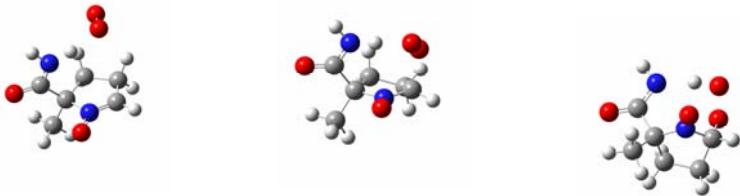
Compound	MSMPO	DEPMPO-3	DEPO Nitrone
file	so2ch3_mpk_n.log	dep-3_mpk_n.log	DEPOb_mpk_n.log
E 6-31+g** tight PCM	-913.670072	-1050.67009	-820.760009
E 6-31+g**	-913.6572619	-1050.676073	-820.7613047
ZPE (raw)	0.177041	0.278495	0.25404
Therm Corr to H (raw)	0.189384	0.297074	0.271754
Therm Corr to G (raw)	0.139724	0.231154	0.208014
H (raw)			
G (raw)			
ZPE (scaled)	0.168455	0.264988	0.241719
Electronic State	1-A	1-A	1-A
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.444000	0.658210	0.70457
Rotational Con. (GHz)	0.946670	0.487310	0.40481
Rotational Con. (GHz)	0.849760	0.336000	0.31709
H298			
6-31+g** tight PCM	-913.489274	-1050.386523	-820.500576
6-31+g**	-913.476464	-1050.392506	-820.501872
G298			
6-31+g** tight PCM	-913.538934	-1050.452443	-820.564316
6-31+g**	-913.526124	-1050.458426	-820.565612



Compound	MAMPO	diMAMPO	diMAPO
file	mampo_mw.log	diMAMPO_3_mw.log	diAmide_mw.log
E 6-31+g** tight PCM	-533.788200	-573.069598	-702.451417
E 6-31+g**	-533.788994	-573.0644375	-702.4500408
ZPE (raw)	0.19517	0.222708	0.222499
Therm Corr to H (raw)	0.20729	0.236431	0.238107
Therm Corr to G (raw)	0.157842	0.183537	0.177586
H (raw)			
G (raw)			
ZPE (scaled)	0.185704	0.211907	0.211708
Electronic State	1-A	1-A	1-A
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.60788	1.52515	0.76149
Rotational Con. (GHz)	0.95756	0.72504	0.6744
Rotational Con. (GHz)	0.83771	0.69832	0.55099
H298			
6-31+g** tight PCM	-533.590376	-572.843968	-702.224101
6-31+g**	-533.591175	-572.838808	-702.222725
G298			
6-31+g** tight PCM	-533.639824	-572.896862	-702.284622
6-31+g**	-533.640623	-572.891702	-702.283246



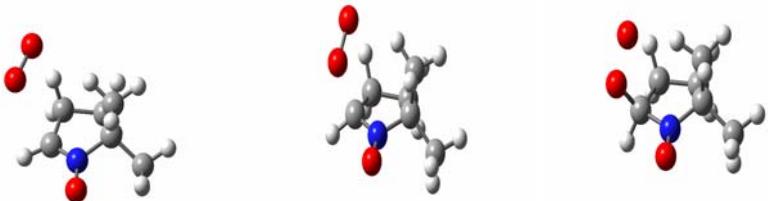
Compound	EMAPO	CPPO-nitrone	Superoxide Radical
file	AMESTmw.log	CPPO.log	superoxideradical_mw.log
E 6-31+g** tight PCM	-722.294459	-442.530852	-150.417388
E 6-31+g**	-722.295606	-442.5280597	-150.3006033
ZPE (raw)	0.210013	0.204585	0.002821
Therm Corr to H (raw)	0.225291	0.2142	0.00614
Therm Corr to G (raw)	0.167771	0.170777	-0.016953
H (raw)			
G (raw)			
ZPE (scaled)	0.199827	0.194663	0.002684
Electronic State	1-A	1-A	—
s2 6-31g*	0	0	0.7564
Symmetry	C1	C1	D*H
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.87919	2.327290	0.000000
Rotational Con. (GHz)	0.64762	1.184470	35.558448
Rotational Con. (GHz)	0.52335	0.996230	35.558448
H298			
6-31+g** tight PCM	-722.079354	-442.326574	-150.411385
6-31+g**	-722.080500	-442.323782	-150.294600
G298			
6-31+g** tight PCM	-722.136874	-442.369997	-150.434478
6-31+g**	-722.138020	-442.367205	-150.317693



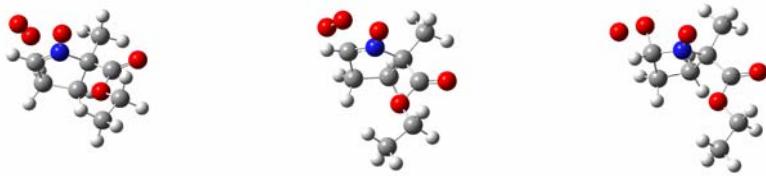
Compound	AMPO-O2 neg	AMPO-O2 TS	AMPO-O2 pos
file	ampO2mpknegF.log	ampO2TSmw.log	ampO2mpk-pos.log
E 6-31+g** tight PCM	-644.915652	-644.900906	-644.930616
E 6-31+g**	-644.831581	-644.812013	-644.847550
ZPE (raw)	0.169819	0.169028	0.171801
Therm Corr to H (raw)	0.183459	0.181457	0.183863
Therm Corr to G (raw)	0.129374	0.131441	0.134519
H (raw)			
G (raw)			
ZPE (scaled)	0.161583	0.160830	0.163469
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.756200	0.805800	0.755100
Symmetry	C1	-	C1
N Imag	0.000000	1 (511.23551)	0.000000
Rotational Con. (GHz)	1.184470	1.275134	1.287460
Rotational Con. (GHz)	0.810170	0.913269	0.933700
Rotational Con. (GHz)	0.655900	0.763523	0.799940
H298			
6-31+g** tight PCM	-644.740429	-644.727647	-644.755085
6-31+g** tight	-644.656358	-644.638754	-644.672020
G298			
6-31+g** tight PCM	-644.794514	-644.777663	-644.804429
6-31+g** tight	-644.710443	-644.688770	-644.721364
E	-1.410641	7.842614	-10.800694
H	-1.357305	6.663750	-10.554164
G	7.307347	17.881737	1.085510



Compound	DEPMPO-O2 neg	DEPMPO-O2 TS	DEPMPO-O2 pos
file	depO2mpk-neg.log	depO2TSmw_4F.log	depO2mpk-pos.log
E 6-31+g** tight PCM	-1201.083726	-1201.066905	-1201.095105
E 6-31+g**	-1201.006343	-1200.998267	-1201.005297
ZPE (raw)	0.281660	0.281374	0.282980
Therm Corr to H (raw)	0.303669	0.301946	0.303804
Therm Corr to G (raw)	0.228206	0.231374	0.232117
H (raw)			
G (raw)			
ZPE (scaled)	0.267999	0.267727	0.269255
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.760900	0.755900	0.757900
Symmetry	C1	C1	C1
N Imag	0.000000	1 (199.2507i)	0.000000
Rotational Con. (GHz)	0.682920	0.596300	0.624370
Rotational Con. (GHz)	0.245620	0.308050	0.302630
Rotational Con. (GHz)	0.203940	0.255690	0.251610
H298			
6-31+g** tight PCM	-1200.793718	-1200.778606	-1200.805026
6-31+g** tight	-1200.716334	-1200.709968	-1200.715218
G298			
6-31+g** tight PCM	-1200.869181	-1200.849178	-1200.876713
6-31+g** tight	-1200.791797	-1200.780540	-1200.786905
E	2.354416	12.909753	-4.786015
H	2.629463	12.112306	-4.466427
G	11.132217	23.684208	6.405803



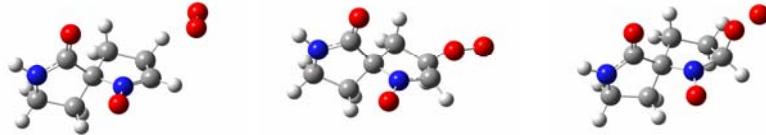
Compound	DMPO-OO C-O neg	DMPO-OO TS	DMPO-OO C-O pos
file	dmpO2mpk-neg.log	dmpoTSmw_2.log	dmpO2mpk-pos.log
E 6-31+g** tight PCM	-515.534471	-515.516044	-515.543919
E 6-31+g**	-515.448525	-515.429245	-515.451847
ZPE (raw)	0.170261	0.169475	0.172407
Therm Corr to H (raw)	0.182776	0.180805	0.183496
Therm Corr to G (raw)	0.130778	0.132960	0.136890
H (raw)			
G (raw)			
ZPE (scaled)	0.162003	0.161255	0.164045
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.759900	0.784600	0.755200
Symmetry	C1	-	C1
N Imag	0.000000	- (611.4438i)	0.000000
Rotational Con. (GHz)	1.998620	1.978193	1.948450
Rotational Con. (GHz)	0.846180	1.119695	1.216000
Rotational Con. (GHz)	0.787170	1.024297	1.128290
H298			
6-31+g** tight PCM	-515.359953	-515.343459	-515.368785
6-31+g** tight	-515.274007	-515.256660	-515.276713
G298			
6-31+g** tight PCM	-515.411951	-515.391304	-515.415391
6-31+g** tight	-515.326005	-515.304505	-515.323319
E	2.773592	14.336710	-3.155118
H	3.070372	13.420590	-2.471843
G	10.424783	23.381048	8.266100



Compound	EMPO-O2 pos	EMPO-O2 TS	EMPO-O2 neg
file	empO2mpk-pos.log	empoO2TSmw.log	empO2mpk-neg.log
E 6-31+g** tight PCM	-743.357925	-743.343885	-743.370606
E 6-31+g**	-743.276839	-743.265139	-743.280002
ZPE (raw)	0.214066	0.213189	0.215602
Therm Corr to H (raw)	0.230935	0.228948	0.231310
Therm Corr to G (raw)	0.167694	0.169416	0.172058
H (raw)			
G (raw)			
ZPE (scaled)	0.203684	0.202849	0.205145
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.761500	0.762000	0.757100
Symmetry	C1	-	C1
N Imag	0.000000	1 (586.4555i)	0.000000
Rotational Con. (GHz)	1.082900	1.114601	1.143520
Rotational Con. (GHz)	0.394310	0.457288	0.461440
Rotational Con. (GHz)	0.355150	0.400860	0.407210
H298			
6-31+g** tight PCM	-743.137372	-743.125277	-743.149753
6-31+g** tight	-743.056287	-743.046530	-743.059149
G298			
6-31+g** tight PCM	-743.200613	-743.184809	-743.209005
6-31+g** tight	-743.119528	-743.106062	-743.118401
E	2.129140	10.939373	-5.828308
H	2.487601	10.077664	-5.281278
G	10.182123	20.099618	4.916379



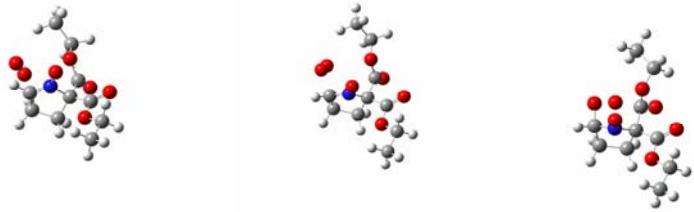
Compound file	CPCOMPO-O2 neg tonO2mpk-neg.log	CPCOMPO-O2 TS tonO2TSmw_2.log	CPCOMPO-O2 pos tonO2mpk-pos.log
E 6-31+g** tight PCM	-702.851440	-702.841099	-702.865250
E 6-31+g**	-702.757277	-702.749288	-702.761038
ZPE (raw)	0.164888	0.164998	0.166680
Therm Corr to H (raw)	0.178571	0.177327	0.178991
Therm Corr to G (raw)	0.122011	0.126055	0.128283
H (raw)			
G (raw)			
ZPE (scaled)	0.156891	0.156996	0.158596
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.760100	0.756200	0.757100
Symmetry	C1	-	C1
N Imag	0.000000	1 (273.88501)	0.000000
Rotational Con. (GHz)	1.572400	1.599308	1.612920
Rotational Con. (GHz)	0.423580	0.548892	0.565040
Rotational Con. (GHz)	0.416870	0.532959	0.544090
H298			
6-31+g** tight PCM	-702.680866	-702.671774	-702.694343
6-31+g** tight	-702.586703	-702.579963	-702.590131
G298			
6-31+g** tight PCM	-702.737426	-702.723046	-702.745051
6-31+g** tight	-702.643263	-702.631235	-702.640839
E	2.666288	9.155364	-5.999618
H	2.823136	8.528243	-5.633754
G	9.720721	18.744097	4.936016



Compound	TAMPO-O2 neg	TAMPO-O2 TS	TAMPO-O2 pos
file	tamO2mpk-neg.log	tamO2TSmw.log	tamO2mpk-pos.log
E 6-31+g** tight PCM	-683.007628	-682.993686	-683.020432
E 6-31+g**	-682.902635	-682.892054	-682.905160
ZPE (raw)	0.177666	0.177341	0.179358
Therm Corr to H (raw)	0.191666	0.189990	0.191921
Therm Corr to G (raw)	0.134745	0.138140	0.140802
H (raw)			
G (raw)			
ZPE (scaled)	0.169049	0.168740	0.170659
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.757600	0.756500	0.756700
Symmetry	C1	-	C1
N Imag	0.000000	1 (333.2348i)	0.000000
Rotational Con. (GHz)	1.568130	1.582951	1.604740
Rotational Con. (GHz)	0.406250	0.549170	0.561810
Rotational Con. (GHz)	0.399380	0.531557	0.540650
H298			
6-31+g** tight PCM	-682.824579	-682.812297	-682.837210
6-31+g** tight	-682.719586	-682.710665	-682.721937
G298			
6-31+g** tight PCM	-682.881500	-682.864147	-682.888329
6-31+g** tight	-682.776507	-682.762515	-682.773056
E	2.813753	11.562490	-5.220879
H	3.064997	10.771920	-4.861114
G	9.908616	20.797639	5.623314



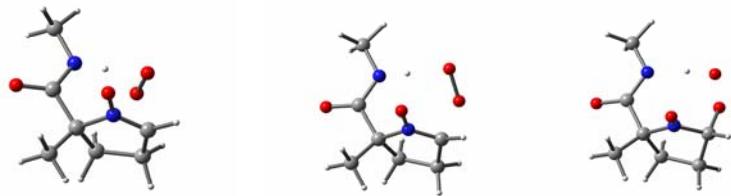
Compound file	TFMPO-O2 neg tfO2mpk-neg.log	TFMPO-O2 TS tfO2TSmw.log	TFMPO-O2 pos tfO2mpk-pos.log
E 6-31+g** tight PCM	-813.203133	-813.192601	-813.216905
E 6-31+g**	-813.123274	-813.113321	-813.128093
ZPE (raw)	0.147426	0.146614	0.148976
Therm Corr to H (raw)	0.161851	0.159990	0.162200
Therm Corr to G (raw)	0.105207	0.106760	0.109583
H (raw)			
G (raw)			
ZPE (scaled)	0.140276	0.139503	0.141751
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.762700	0.759700	0.757400
Symmetry	C1	-	C1
N Imag	0.000000	1 (535.6201i)	0.000000
Rotational Con. (GHz)	1.433050	1.520662	1.532620
Rotational Con. (GHz)	0.495920	0.549205	0.571130
Rotational Con. (GHz)	0.465370	0.513715	0.534200
H298			
6-31+g** tight PCM	-813.048432	-813.039722	-813.061930
6-31+g** tight	-812.968573	-812.960442	-812.973118
G298			
6-31+g** tight PCM	-813.105076	-813.092952	-813.114547
6-31+g** tight	-813.025217	-813.013672	-813.025735
E	2.033758	8.642688	-6.608303
H	2.500871	7.966719	-5.969362
G	10.343485	17.951650	4.400233



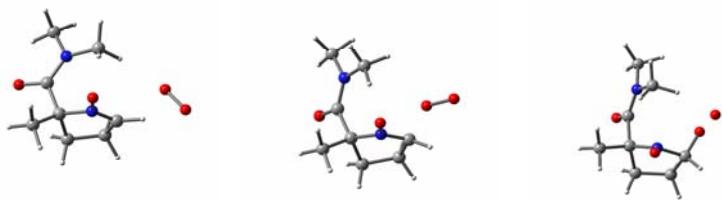
Compound	DEPO-OO pos	DEPO-OO TS	DEPO-OO neg
file	DEPO-O2mpk-pos.log	DEPO-O2TSmwF_n.log	DEPO-O2mpk-negF.log
E 6-31+g** tight PCM	-971.172688	-971.158762	-971.193084
E 6-31+g**	-971.099252	-971.084539	-971.117769
ZPE (raw)	0.257518	0.256395	0.259912
Therm Corr to H (raw)	0.278483	0.276511	0.278749
Therm Corr to G (raw)	0.206566	0.205979	0.212383
H (raw)			
G (raw)			
ZPE (scaled)	0.245028	0.243960	0.247306
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.760300	0.756000	0.755100
Symmetry	C1	C1	C1
N Imag	0.000000	1 (917.2002i)	0.000000
Rotational Con. (GHz)	0.732700	0.585855	0.612760
Rotational Con. (GHz)	0.275250	0.335090	0.359290
Rotational Con. (GHz)	0.243730	0.274934	0.291180
H298			
6-31+g** tight PCM	-970.906695	-970.894686	-970.926941
6-31+g** tight	-970.833259	-970.820463	-970.851626
G298			
6-31+g** tight PCM	-970.978612	-970.965218	-970.993307
6-31+g** tight	-970.905176	-970.890995	-970.917992
E	2.954942	11.693640	-9.843742
H	3.304550	10.839976	-9.400076
G	12.664482	21.069009	3.443161



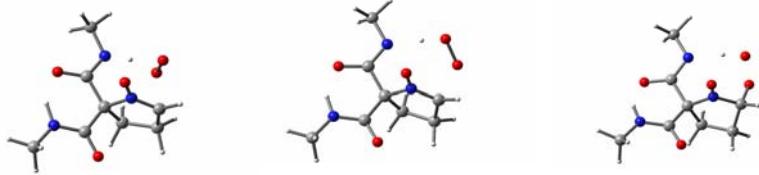
Compound	CPPO-OO neg	CPPO-OO	CPPO-OO pos
file	CPP-OOmPK-neg.log	CPPO-OO.log	CPP-OOmPK-pos.log
E 6-31+g** tight PCM	-592.943416	-592.927467	-592.955732
E 6-31+g**	-592.854782	-592.840662	-592.840662
ZPE (raw)	0.207666	0.206787	0.209228
Therm Corr to H (raw)	0.220929	0.218848	0.221311
Therm Corr to G (raw)	0.166186	0.168360	0.170628
H (raw)			
G (raw)			
ZPE (scaled)	0.197594	0.196758	0.199080
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.760500	0.764100	0.756700
Symmetry	C1	C1	C1
N Imag	0.000000	1 (638.6218i)	0.000000
Rotational Con. (GHz)	1.913660	1.962340	2.029660
Rotational Con. (GHz)	0.497700	0.614490	0.624150
Rotational Con. (GHz)	0.468660	0.577980	0.583890
H298			
6-31+g** tight PCM	-592.732559	-592.718648	-592.744569
6-31+g** tight	-592.643924	-592.631843	-592.629498
G298			
6-31+g** tight PCM	-592.787302	-592.769136	-592.795252
6-31+g** tight	-592.698667	-592.682331	-592.680181
E	3.027106	13.035255	-4.701301
H	3.388796	12.117849	-4.147441
G	10.776465	22.175572	5.787917



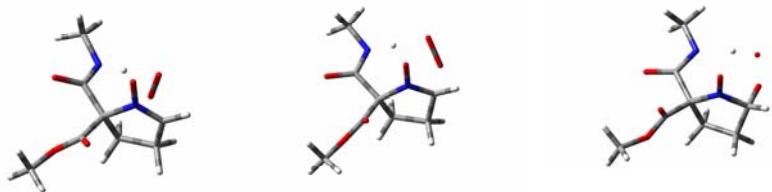
Compound	MAMPO-OO neg	MAMPO-OO TS	MAMPO-OO pos
file	neg- MAMPO_O2TSmw.log	pos- MAMPOcis_O2TSmw.log	pos- MAMPO_O2mw.log
E 6-31+g** tight PCM	-684.208458	-684.193339	-684.219856
E 6-31+g**	-684.132279	-684.112475	-684.146524
ZPE (raw)	0.197930	0.197158	0.199138
Therm Corr to H (raw)	0.213346	0.211354	0.212908
Therm Corr to G (raw)	0.155146	0.157205	0.159753
H (raw)			
G (raw)			
ZPE (scaled)	0.188330	0.187596	0.189480
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.756300	0.805400	0.755100
Symmetry	C1	C1	C1
N Imag	0.000000	1 (513.4450i)	0.000000
Rotational Con. (GHz)	0.892010	0.976530	1.019190
Rotational Con. (GHz)	0.787910	0.844720	0.836510
Rotational Con. (GHz)	0.557640	0.615030	0.634680
H298			
6-31+g** tight PCM	-684.004712	-683.991547	-684.016606
6-31+g** tight	-683.928532	-683.910684	-683.943274
G298			
6-31+g** tight PCM	-684.062912	-684.045696	-684.069761
6-31+g** tight	-683.986732	-683.964833	-683.996429
E	-1.800952	7.686364	-8.953306
H	-1.851807	6.409006	-9.315774
G	7.147307	17.950161	2.849126



Compound	DIMAMPO-OO neg neg- Dimam_O2TSmw.log	DIMAMPO-OO TS diMAMPO- O2_cisTSmw.log	DIMAMPO-OO pos pos- Dimam_O2TSmw.log
E 6-31+g** tight PCM	-723.483279	-723.469350	-723.497095
E 6-31+g**	-723.406452	-723.396950	-723.410880
ZPE (raw)	0.227010	0.225938	0.228408
Therm Corr to H (raw)	0.243701	0.241523	0.243894
Therm Corr to G (raw)	0.182914	0.183803	0.186797
H (raw)			
G (raw)			
ZPE (scaled)	0.216000	0.214980	0.217330
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.759500	0.756700	0.755300
Symmetry	C1	C1	C1
N Imag	0.000000	1 (265.4428i)	0.000000
Rotational Con. (GHz)	0.887490	0.857290	0.838410
Rotational Con. (GHz)	0.543100	0.642780	0.729990
Rotational Con. (GHz)	0.443140	0.527380	0.594460
H298			
6-31+g** tight PCM	-723.250588	-723.238785	-723.264279
6-31+g** tight	-723.173761	-723.166385	-723.178064
G298			
6-31+g** tight PCM	-723.311375	-723.296505	-723.321376
6-31+g** tight	-723.234548	-723.224105	-723.235161
E	2.326178	11.066758	-6.343494
H	2.990190	10.396680	-5.600919
G	12.528335	21.859396	6.252736



Compound	DIMAPO-OO neg	DIMAPO-OO TS	DIMAPO-OO pos
file	neg-diMAPO_O2mw.log	diMAPO_O2_mw_a.log	pos-diMAPO_O2mw.log
E 6-31+g** tight PCM	-852.873234	-852.852653	-852.889850
E 6-31+g**	-852.802315	-852.783900	-852.821431
ZPE (raw)	0.225057	0.223950	0.227295
Therm Corr to H (raw)	0.243579	0.241087	0.244279
Therm Corr to G (raw)	0.177410	0.179278	0.182870
H (raw)			
G (raw)			
ZPE (scaled)	0.214142	0.213088	0.216271
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.756100	0.821400	0.754700
Symmetry	C1	C1	C1
N Imag	0.000000	1 (449.7613i)	0.000000
Rotational Con. (GHz)	0.780910	0.774760	0.772290
Rotational Con. (GHz)	0.424640	0.480080	0.492820
Rotational Con. (GHz)	0.342570	0.358590	0.368420
H298			
6-31+g** tight PCM	-852.640570	-852.622428	-852.656595
6-31+g** tight	-852.569651	-852.553674	-852.588176
G298			
6-31+g** tight PCM	-852.706739	-852.684237	-852.718004
6-31+g** tight	-852.635820	-852.615483	-852.649585
E	-2.779240	10.135533	-13.205937
H	-3.190412	8.194298	-13.245965
G	7.756492	21.877143	0.687884



Compound	EMAPO-OO neg	EMAPO-OO TS	EMAPO-OO pos
	pos- EMAPO_O2mw.log	pos- EMAPO_O2mw.log	pos- EMAPO_O2mw.log
file	neg-EMAPO_O2mw.log	EMAPO_O2_mw.log	EMAPO_O2mw.log
E 6-31+g** tight PCM	-872.715297	-872.699194	-872.727294
E 6-31+g**	-872.639807	-872.619123	-872.654279
ZPE (raw)	0.212444	0.211409	0.214238
Therm Corr to H (raw)	0.231010	0.228666	0.231138
Therm Corr to G (raw)	0.164901	0.166774	0.169687
H (raw)			
G (raw)			
ZPE (scaled)	0.202140	0.201156	0.203847
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.756300	0.812500	0.754800
Symmetry	C1	C1	C1
N Imag	0.000000	1 (515.9052i)	0.000000
Rotational Con. (GHz)	0.721970	0.790280	0.789920
Rotational Con. (GHz)	0.426020	0.468440	0.475180
Rotational Con. (GHz)	0.368910	0.372460	0.381550
H298			
6-31+g** tight PCM	-872.494591	-872.480781	-872.506547
6-31+g** tight	-872.419101	-872.400710	-872.433532
G298			
6-31+g** tight PCM	-872.560700	-872.542673	-872.567998
6-31+g** tight	-872.485210	-872.462602	-872.494983
E	-2.164908	7.939878	-9.693139
H	-2.417220	6.248183	-9.919729
G	6.684178	17.995788	2.104608

PCM-CH3CN/mpw1pw91/6-31+g**

ZPE scaling factor =

0.9515000

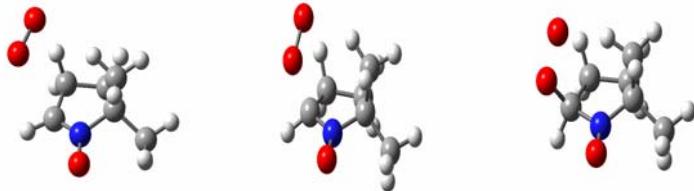
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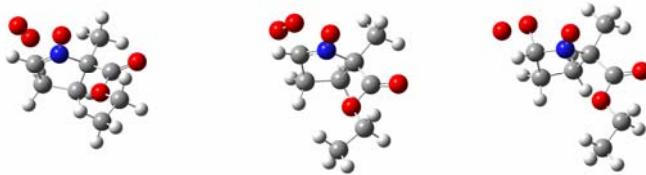
Compound	AMPO-O2 neg	AMPO-O2 TS	AMPO-O2 pos
file	ampO2mpknegF.log	ampO2TSmw.log	ampO2mpk-pos.log
E 6-31+g** tight PCM	-644.9128800	-644.8978020	-644.9274720
E 6-31+g**	-644.8315807	-644.8120131	-644.8475503
ZPE (raw)	0.1698190	0.1690280	0.1718010
Therm Corr to H (raw)	0.1834590	0.1814570	0.1838630
Therm Corr to G (raw)	0.1293740	0.1314410	0.1345190
H (raw)			
G (raw)			
ZPE (scaled)	0.1615828	0.1608301	0.1634687
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7562000	0.8058000	0.7551000
Symmetry	C1	-	C1
N Imag	0.0000000	1 (511.2355i)	0.0000000
Rotational Con. (GHz)	1.1844700	1.2751343	1.2874600
Rotational Con. (GHz)	0.8101700	0.9132690	0.9337000
Rotational Con. (GHz)	0.6559000	0.7635230	0.7999400
H298			
6-31+g** tight PCM	-644.7376572	-644.7245429	-644.7519413
6-31+g** tight	-644.6563580	-644.6387540	-644.6720196
G298			
6-31+g** tight PCM	-644.7917422	-644.7745589	-644.8012853
6-31+g** tight	-644.7104430	-644.6887700	-644.7213636
E	-1.6986682	7.7629200	-10.8552868
H	-1.6453315	6.5840562	-10.6087569
G	7.0193197	17.8020435	1.0309168



Compound	DEPMPO-O2 neg	DEPMPO-O2 TS	DEPMPO-O2 pos
file	depO2mpk-neg.log	depO2TSmw_4F.log	depO2mpk-pos.log
E 6-31+g** tight PCM	-1201.0815890	-1201.0638580	-1201.0923260
E 6-31+g**	-1201.0063426	-1200.9982674	-1201.0052973
ZPE (raw)	0.2816600	0.2813740	0.2829800
Therm Corr to H (raw)	0.3036690	0.3019460	0.3038040
Therm Corr to G (raw)	0.2282060	0.2313740	0.2321170
H (raw)			
G (raw)			
ZPE (scaled)	0.2679995	0.2677274	0.2692555
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7609000	0.7559000	0.7579000
Symmetry	C1	C1	C1
N Imag	0.0000000	1 (199.2507i)	0.0000000
Rotational Con. (GHz)	0.6829200	0.5963000	0.6243700
Rotational Con. (GHz)	0.2456200	0.3080500	0.3026300
Rotational Con. (GHz)	0.2039400	0.2556900	0.2516100
H298			
6-31+g** tight PCM	-1200.7915805	-1200.7755586	-1200.8022465
6-31+g** tight	-1200.7163341	-1200.7099680	-1200.7152178
G298			
6-31+g** tight PCM	-1200.8670435	-1200.8461306	-1200.8739335
6-31+g** tight	-1200.7917971	-1200.7805400	-1200.7869048
E	2.3788885	13.5052595	-4.3586810
H	2.6539360	12.7078122	-4.0390929
G	11.1566897	24.2797149	6.8331367



Compound	DMPO-OO C-O neg	DMPO-OO TS	DMPO-OO C-O pos
file	dmpO2mpk-neg.log	dmpoTSmw_2.log	dmpO2mpk-pos.log
E 6-31+g** tight PCM	-515.5319800	-515.5130340	-515.5411250
E 6-31+g**	-515.4485250	-515.4292450	-515.4518474
ZPE (raw)	0.1702610	0.1694750	0.1724070
Therm Corr to H (raw)	0.1827760	0.1808050	0.1834960
Therm Corr to G (raw)	0.1307780	0.1329600	0.1368900
H (raw)			
G (raw)			
ZPE (scaled)	0.1620033	0.1612555	0.1640453
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7599000	0.7846000	0.7552000
Symmetry	C1	-	C1
N Imag	0.0000000	- (611.4438i)	0.0000000
Rotational Con. (GHz)	1.9986200	1.9781928	1.9484500
Rotational Con. (GHz)	0.8461800	1.1196951	1.2160000
Rotational Con. (GHz)	0.7871700	1.0242967	1.1282900
H298			
6-31+g** tight PCM	-515.3574617	-515.3404485	-515.3659907
6-31+g** tight	-515.2740067	-515.2566595	-515.2767131
G298			
6-31+g** tight PCM	-515.4094597	-515.3882935	-515.4125967
6-31+g** tight	-515.3260047	-515.3045045	-515.3233191
E	2.7773570	14.6661520	-2.9612173
H	3.0741370	13.7500321	-2.2779423
G	10.4285484	23.7104904	8.4600002



Compound	EMPO-O2 pos	EMPO-O2 TS	EMPO-O2 neg
file	empO2mpk-pos.log	empoO2TSmw.log	empO2mpk-neg.log
E 6-31+g** tight PCM	-743.3555300	-743.3415960	-743.3679340
E 6-31+g**	-743.2768394	-743.2651387	-743.2800025
ZPE (raw)	0.2140660	0.2131890	0.2156020
Therm Corr to H (raw)	0.2309350	0.2289480	0.2313100
Therm Corr to G (raw)	0.1676940	0.1694160	0.1720580
H (raw)			
G (raw)			
ZPE (scaled)	0.2036838	0.2028493	0.2051453
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7615000	0.7620000	0.7571000
Symmetry	C1	-	C1
N Imag	0.0000000	1 (586.4555i)	0.0000000
Rotational Con. (GHz)	1.0829000	1.1146011	1.1435200
Rotational Con. (GHz)	0.3943100	0.4572884	0.4614400
Rotational Con. (GHz)	0.3551500	0.4008599	0.4072100
H298			
6-31+g** tight PCM	-743.1349772	-743.1229877	-743.1470807
6-31+g** tight	-743.0562866	-743.0465304	-743.0591492
G298			
6-31+g** tight PCM	-743.1982182	-743.1825197	-743.2063327
6-31+g** tight	-743.1195276	-743.1060624	-743.1184012
E	2.1090594	10.8527768	-5.6745684
H	2.4675208	9.9910676	-5.1275379
G	10.1620423	20.0130218	5.0701189



Compound	MCCP-O2 neg	MCCP-O2 TS	MCCP-O2 pos
file	neg-MCCP_O2.log	MCCP-O2-TS-mPW1K.log	pos-MCCP_O2.log
E 6-31+g** tight PCM	-554.9356580	-554.9349430	-554.9370320
E 6-31+g**	-554.8606175	-554.8587111	-554.8602272
ZPE (raw)	0.2005500	0.2001560	0.2007050
Therm Corr to H (raw)	0.2139650	0.2128080	0.2140980
Therm Corr to G (raw)	0.1602530	0.1603540	0.1597250
H (raw)			
G (raw)			
ZPE (scaled)	0.1908233	0.1904484	0.1909708
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7563000	0.7563000	0.7563000
Symmetry	C1	C1	C1
N Imag	0.0000000	1 (26.8798i)	0.0000000
Rotational Con. (GHz)	1.5069700	1.4554800	1.5847800
Rotational Con. (GHz)	0.7473200	0.7357800	0.6719300
Rotational Con. (GHz)	0.6642400	0.6242300	0.5572500
H298			
6-31+g** tight PCM	-554.7314197	-554.7318426	-554.7326682
6-31+g** tight	-554.6563792	-554.6556107	-554.6558634
G298			
6-31+g** tight PCM	-554.7851317	-554.7842966	-554.7870412
6-31+g** tight	-554.7100912	-554.7080647	-554.7102364
E	-4.6670241	-4.2183548	-5.5292221
H	-3.2929107	-3.5582788	-4.0763673
G	5.8938284	6.4178672	4.6955880

Compound	Superoxide Radical	AMPO	EMPO-1
file	superoxideradical_mw.log	conh2_mpk_n.log	empocis_mpk_n.log
E 6-31+g** tight PCM	-150.4154420	-494.4947310	-592.9434490
E 6-31+g**	-150.3006033	-494.4878752	-592.9445344
ZPE (raw)	0.0028210	0.1668330	0.2109820
Therm Corr to H (raw)	0.0061400	0.1772260	0.2242110
Therm Corr to G (raw)	-0.0169530	0.1324260	0.1718010
H (raw)			
G (raw)			
ZPE (scaled)	0.0026842	0.1587416	0.2007494
Electronic State	—	1-A	1-A
s2 6-31g*	0.7564000	0.0000000	0.0000000
Symmetry	D*H	C1	C1
N Imag	0.0000000	0.0000000	0.0000000
Rotational Con. (GHz)	0.0000000	1.7698100	1.3976400
Rotational Con. (GHz)	35.5584482	1.3896500	0.7359900
Rotational Con. (GHz)	35.5584482	1.1283800	0.6676100
H298			
6-31+g** tight PCM	-150.4094388	-494.3255964	-592.7294706
6-31+g** tight	-150.2946001	-494.3187406	-592.7305561
G298			
6-31+g** tight PCM	-150.4325318	-494.3703964	-592.7818806
6-31+g** tight	-150.3176931	-494.3635406	-592.7829661
Compound	DMPO	DEPMPO-3	MCCP
file	dmpo1_mpk_n.log	dep-3_mpk_n.log	MCCP_mpw1k.log
E 6-31+g** tight PCM	-365.1209640	-1050.6699380	-404.5149110
E 6-31+g**	-365.1206901	-1050.6760734	-404.5127786
ZPE (raw)	0.1672740	0.2784950	0.1973870
Therm Corr to H (raw)	0.1761550	0.2970740	0.2077510
Therm Corr to G (raw)	0.1355300	0.2311540	0.1624920
H (raw)			
G (raw)			
ZPE (scaled)	0.1591612	0.2649880	0.1878137
Electronic State	1-A	1-A	1-A
s2 6-31g*	0.0000000	0.0000000	0.0000000
Symmetry	C1	C1	C1
N Imag	0.0000000	0.0000000	0.0000000
Rotational Con. (GHz)	2.6357800	0.6582100	2.5898000
Rotational Con. (GHz)	2.2772300	0.4873100	1.3394000
Rotational Con. (GHz)	1.6874200	0.3360000	1.1636500
H298			
6-31+g** tight PCM	-364.9529218	-1050.3863710	-404.3167333
6-31+g** tight	-364.9526479	-1050.3925064	-404.3146009
G298			
6-31+g** tight PCM	-364.9935468	-1050.4522910	-404.3619923
6-31+g** tight	-364.9932729	-1050.4584264	-404.3598599

PCM-DMSO/mpw1pw91/6-31+g**

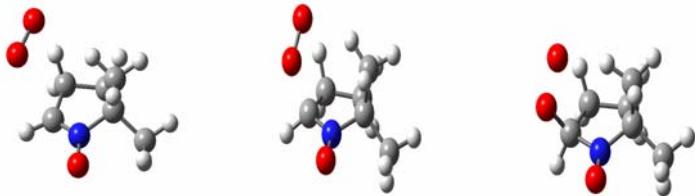
ZPE scaling factor = 0.9515000 hartree to kcal/mol =



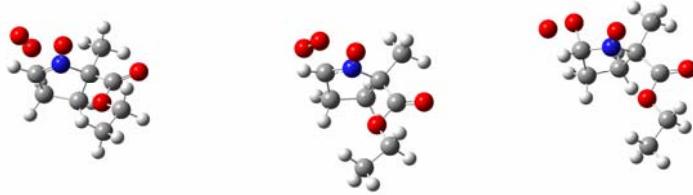
Compound	AMPO-O2 neg	AMPO-O2 TS	AMPO-O2 pos
file	ampO2mpknegF.log	ampO2TSmw.log	ampO2mpk-pos.log
E 6-31+g** tight PCM	-644.9170330	-644.9021310	-644.9320900
E 6-31+g**	-644.8315807	-644.8120131	-644.8475503
ZPE (raw)	0.1698190	0.1690280	0.1718010
Therm Corr to H (raw)	0.1834590	0.1814570	0.1838630
Therm Corr to G (raw)	0.1293740	0.1314410	0.1345190
H (raw)			
G (raw)			
ZPE (scaled)	0.1615828	0.1608301	0.1634687
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7562000	0.8058000	0.7551000
Symmetry	C1	-	C1
N Imag	0.0000000	1 (511.2355i)	0.0000000
Rotational Con. (GHz)	1.1844700	1.2751343	1.2874600
Rotational Con. (GHz)	0.8101700	0.9132690	0.9337000
Rotational Con. (GHz)	0.6559000	0.7635230	0.7999400
H298			
6-31+g** tight PCM	-644.7418102	-644.7288719	-644.7565593
6-31+g** tight	-644.6563580	-644.6387540	-644.6720196
G298			
6-31+g** tight PCM	-644.7958952	-644.7788879	-644.8059033
6-31+g** tight	-644.7104430	-644.6887700	-644.7213636
E	-1.2506264	8.1005201	-10.6990370
H	-1.1972897	6.9216563	-10.4525070
G	7.4673615	18.1396436	1.1871667



Compound	DEPMPO-O2 neg	DEPMPO-O2 TS	DEPMPO-O2 pos
file	depO2mpk-neg.log	depO2TSmw_4F.log	depO2mpk-pos.log
E 6-31+g** tight PCM	-1201.0865940	-1201.0689940	-1201.0975130
E 6-31+g**	-1201.0063426	-1200.9982674	-1201.0052973
ZPE (raw)	0.2816600	0.2813740	0.2829800
Therm Corr to H (raw)	0.3036690	0.3019460	0.3038040
Therm Corr to G (raw)	0.2282060	0.2313740	0.2321170
H (raw)			
G (raw)			
ZPE (scaled)	0.2679995	0.2677274	0.2692555
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7609000	0.7559000	0.7579000
Symmetry	C1	C1	C1
N Imag	0.0000000	1 (199.2507i)	0.0000000
Rotational Con. (GHz)	0.6829200	0.5963000	0.6243700
Rotational Con. (GHz)	0.2456200	0.3080500	0.3026300
Rotational Con. (GHz)	0.2039400	0.2556900	0.2516100
H298			
6-31+g** tight PCM	-1200.7965855	-1200.7806946	-1200.8074335
6-31+g** tight	-1200.7163341	-1200.7099680	-1200.7152178
G298			
6-31+g** tight PCM	-1200.8720485	-1200.8512666	-1200.8791205
6-31+g** tight	-1200.7917971	-1200.7805400	-1200.7869048
E	2.8030849	13.8472521	-4.0486913
H	3.0781324	13.0498049	-3.7291032
G	11.5808861	24.6217076	7.1431264



Compound	DMPO-OO C-O neg	DMPO-OO TS	DMPO-OO C-O pos
file	dmpO2mpk-neg.log	dmpoTSmw_2.log	dmpO2mpk-pos.log
E 6-31+g** tight PCM	-515.5357120	-515.5169890	-515.5452180
E 6-31+g**	-515.4485250	-515.4292450	-515.4518474
ZPE (raw)	0.1702610	0.1694750	0.1724070
Therm Corr to H (raw)	0.1827760	0.1808050	0.1834960
Therm Corr to G (raw)	0.1307780	0.1329600	0.1368900
H (raw)			
G (raw)			
ZPE (scaled)	0.1620033	0.1612555	0.1640453
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7599000	0.7846000	0.7552000
Symmetry	C1	-	C1
N Imag	0.0000000	- (611.4438i)	0.0000000
Rotational Con. (GHz)	1.9986200	1.9781928	1.9484500
Rotational Con. (GHz)	0.8461800	1.1196951	1.2160000
Rotational Con. (GHz)	0.7871700	1.0242967	1.1282900
H298			
6-31+g** tight PCM	-515.3611937	-515.3444035	-515.3700837
6-31+g** tight	-515.2740067	-515.2566595	-515.2767131
G298			
6-31+g** tight PCM	-515.4131917	-515.3922485	-515.4166897
6-31+g** tight	-515.3260047	-515.3045045	-515.3233191
E	3.3521557	15.1010161	-2.6129496
H	3.6489357	14.1848962	-1.9296745
G	11.0033471	24.1453545	8.8082680



Compound	EMPO-O2 pos	EMPO-O2 TS	EMPO-O2 neg
file	empO2mpk-pos.log	empoO2TSmw.log	empO2mpk-neg.log
E 6-31+g** tight PCM	-743.3596880	-743.3459450	-743.3725230
E 6-31+g**	-743.2768394	-743.2651387	-743.2800025
ZPE (raw)	0.2140660	0.2131890	0.2156020
Therm Corr to H (raw)	0.2309350	0.2289480	0.2313100
Therm Corr to G (raw)	0.1676940	0.1694160	0.1720580
H (raw)			
G (raw)			
ZPE (scaled)	0.2036838	0.2028493	0.2051453
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7615000	0.7620000	0.7571000
Symmetry	C1	-	C1
N Imag	0.0000000	1 (586.4555i)	0.0000000
Rotational Con. (GHz)	1.0829000	1.1146011	1.1435200
Rotational Con. (GHz)	0.3943100	0.4572884	0.4614400
Rotational Con. (GHz)	0.3551500	0.4008599	0.4072100
H298			
6-31+g** tight PCM	-743.1391352	-743.1273367	-743.1516697
6-31+g** tight	-743.0562866	-743.0465304	-743.0591492
G298			
6-31+g** tight PCM	-743.2023762	-743.1868687	-743.2109217
6-31+g** tight	-743.1195276	-743.1060624	-743.1184012
E	2.7146061	11.3384692	-5.3394783
H	3.0730674	10.4767599	-4.7924479
G	10.7675889	20.4987142	5.4052090



Compound	MCCP-O2 neg	MCCP-O2 TS	MCCP-O2 pos
file	neg-MCCP_O2.log	MCCP-O2-TS-mPW1K.log	pos-MCCP_O2.log
E 6-31+g** tight PCM	-554.9401560	-554.9391970	-554.9414150
E 6-31+g**	-554.8606175	-554.8587111	-554.8602272
ZPE (raw)	0.2005500	0.2001560	0.2007050
Therm Corr to H (raw)	0.2139650	0.2128080	0.2140980
Therm Corr to G (raw)	0.1602530	0.1603540	0.1597250
H (raw)			
G (raw)			
ZPE (scaled)	0.1908233	0.1904484	0.1909708
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7563000	0.7563000	0.7563000
Symmetry	C1	C1	C1
N Imag	0.0000000	1 (26.8798i)	0.0000000
Rotational Con. (GHz)	1.5069700	1.4554800	1.5847800
Rotational Con. (GHz)	0.7473200	0.7357800	0.6719300
Rotational Con. (GHz)	0.6642400	0.6242300	0.5572500
H298			
6-31+g** tight PCM	-554.7359177	-554.7360966	-554.7370512
6-31+g** tight	-554.6563792	-554.6556107	-554.6558634
G298			
6-31+g** tight PCM	-554.7896297	-554.7885506	-554.7914242
6-31+g** tight	-554.7100912	-554.7080647	-554.7102364
E	-6.5627303	-5.9609487	-7.3527648
H	-2.7996882	-2.9119440	-3.5109812
G	6.3870509	7.0642020	5.2609741

Compound	Superoxide Radical	AMPO	DEPMPO-3
file	superoxideradical_mw.log	conh2_mpk_n.log	dep-3_mpk_n.log
E 6-31+g** tight PCM	-150.4169190	-494.4981210	-1050.6741420
E 6-31+g**	-150.3006033	-494.4878752	-1050.6760734
ZPE (raw)	0.0028210	0.1668330	0.2784950
Therm Corr to H (raw)	0.0061400	0.1772260	0.2970740
Therm Corr to G (raw)	-0.0169530	0.1324260	0.2311540
H (raw)			
G (raw)			
ZPE (scaled)	0.0026842	0.1587416	0.2649880
Electronic State	—	1-A	1-A
s2 6-31g*	0.7564000	0.0000000	0.0000000
Symmetry	D*H	C1	C1
N Imag	0.0000000	0.0000000	0.0000000
Rotational Con. (GHz)	0.0000000	1.7698100	0.6582100
Rotational Con. (GHz)	35.5584482	1.3896500	0.4873100
Rotational Con. (GHz)	35.5584482	1.1283800	0.3360000
H298			
6-31+g** tight PCM	-150.4109158	-494.3289864	-1050.3905750
6-31+g** tight	-150.2946001	-494.3187406	-1050.3925064
G298			
6-31+g** tight PCM	-150.4340088	-494.3737864	-1050.4564950
6-31+g** tight	-150.3176931	-494.3635406	-1050.4584264
 Compound	 DMPO	 EMPO-1	 MCCP
file	dmpo1_mpk_n.log	empocis_mpk_n.log	MCCP_mpw1k.log
E 6-31+g** tight PCM	-365.1241350	-592.9470950	-404.5187180
E 6-31+g**	-365.1206901	-592.9445344	-404.5127786
ZPE (raw)	0.1672740	0.2109820	0.1973870
Therm Corr to H (raw)	0.1761550	0.2242110	0.2077510
Therm Corr to G (raw)	0.1355300	0.1718010	0.1624920
H (raw)			
G (raw)			
ZPE (scaled)	0.1591612	0.2007494	0.1878137
Electronic State	1-A	1-A	1-A
s2 6-31g*	0.0000000	0.0000000	0.0000000
Symmetry	C1	C1	C1
N Imag	0.0000000	0.0000000	0.0000000
Rotational Con. (GHz)	2.6357800	1.3976400	2.5898000
Rotational Con. (GHz)	2.2772300	0.7359900	1.3394000
Rotational Con. (GHz)	1.6874200	0.6676100	1.1636500
H298			
6-31+g** tight PCM	-364.9560928	-592.7331166	-404.3205403
6-31+g** tight	-364.9526479	-592.7305561	-404.3146009
G298			
6-31+g** tight PCM	-364.9967178	-592.7855266	-404.3657993
6-31+g** tight	-364.9932729	-592.7829661	-404.3598599

Table S9. Thermodynamic parameters at the PCM-B3LYP/6-31+Glevel of theory.**

Compound	Superoxide PCM	AMPO PCM	AMPO-O2 TS PCM
file	O2_opt_pcmb3lyp.log	AMPO_opt_pcmb3lyp.log	AMPO_O2_TSpcmopt.log
E 6-31+g** tight PCM	-150.465109	-494.615441	-645.067638
E 6-31+g**	-150.465109	-494.615441	-645.067638
ZPE (raw)	0.002728	0.163261	0.167319
Therm Corr to H (raw)	0.00605	0.173853	0.179971
Therm Corr to G (raw)	-0.017067	0.128593	0.129537
H (raw)			
G (raw)			
ZPE (scaled)	0.002675	0.160094	0.164073
Electronic State	–	1-A	2-A
s2 6-31g*	0.756	0	0.7855
Symmetry	D*H	C1	C1
N Imag	0.000000	0.000000	1 (518.5157i)
Rotational Con. (GHz)	0	1.75705	1.26291
Rotational Con. (GHz)	34.7782877	1.34861	0.89081
Rotational Con. (GHz)	34.7782877	1.10853	0.742
H298			
6-31+g** tight PCM	-150.459112	-494.444755	-644.890913
6-31+g**	-150.459112	-494.444755	-644.890913
G298			
6-31+g** tight PCM	-150.482229	-494.490015	-644.941347
6-31+g**	-150.482229	-494.490015	-644.941347
Compound	DMPO PCM	DMPO-O2 TS PCM	
file	DMPO_opt_pcmb3lyp.log	DMPO_O2_TSpcmopt.log	
E 6-31+g** tight PCM	-365.209372	-515.653456	
E 6-31+g**	-365.209372	-515.653456	
ZPE (raw)	0.164952	0.167803	
Therm Corr to H (raw)	0.173906	0.179394	
Therm Corr to G (raw)	0.133138	0.131015	
H (raw)			
G (raw)			
ZPE (scaled)	0.161752	0.164548	
Electronic State	1-A	2-A	
s2 6-31g*	0	0.7829	
Symmetry	C1	C1	
N Imag	0.000000	1 (648.7148i)	
Rotational Con. (GHz)	2.57231	2.09135	
Rotational Con. (GHz)	2.25421	0.9908	
Rotational Con. (GHz)	1.65612	0.89065	
H298			
6-31+g** tight PCM	-365.038666	-515.477317	
6-31+g**	-365.038666	-515.477317	
G298			
6-31+g** tight PCM	-365.079434	-515.525696	
6-31+g**	-365.079434	-515.525696	

Table S10. Thermodynamic parameters for compounds found in Scheme 2 at the PCM/B3LYP/6-31+G//B3LYP/6-31G* level of theory.**

PCM/b3lyp/6-31+g**//b3lyp/6-31g*

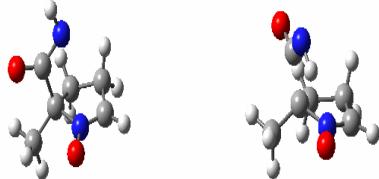
ZPE scaling factor =

0.9806

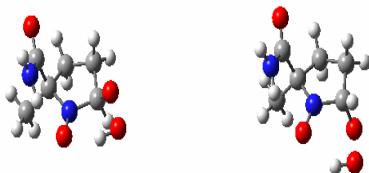
hartree to kcal/mol =



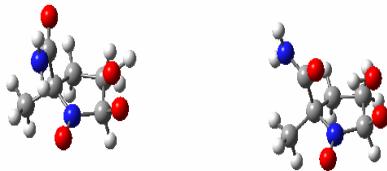
Compound file	OOH Radical peroxyrad.log	O2 Radical o2.log	AMPO conh2.log
E 6-31+g** PCM	-150.926851	-150.465075	-494.613836
E 6-31g*	-150.899156	-150.2996938	-494.5653155
ZPE (raw)	0.014031	0.002761	0.166017
Therm Corr to H (raw)	0.017832	0.006082	0.176458
Therm Corr to G (raw)	-0.008160	-0.017041	0.13143
H (raw)	-150.881325	-150.293612	-494.388857
G (raw)	-150.907317	-150.316735	-494.433885
ZPE (scaled)	0.013759	0.002707	0.162796
Electronic State			
s2 6-31g*	0.752700	0.7528	0.000000
Symmetry	C01	C01	C01
N Imag	0.000000	0	0.000000
Rotational Con. (GHz)		1.63425	1.755748
Rotational Con. (GHz)		0.75785	1.375520
Rotational Con. (GHz)		0.66048	1.109713
H298			
H 6-31+g** PCM	-150.909291	-150.459047	-494.440599
H 6-31g*	-150.881597	-150.293665	-494.392078
G298			
G 6-31+g** PCM	-150.935283	-150.482170	-494.485627
G 6-31g*	-150.907589	-150.316788	-494.437106



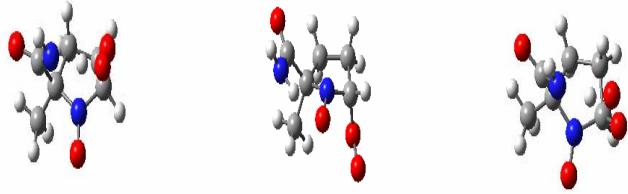
Compound	AMPO-NH a	AMPO-NH b
file	AMPOneg1.log	AMPOneg2.log
E 6-31+g** PCM	-494.113534	-494.11361
E 6-31g*	-493.9666042	-493.9612699
ZPE (raw)	0.151687	0.151502
Therm Corr to H (raw)	0.161944	0.161786
Therm Corr to G (raw)	0.116655	0.116629
H (raw)	-493.80466	-493.799484
G (raw)	-493.849949	-493.844641
ZPE (scaled)	0.148744	0.148563
Electronic State		
s2 6-31g*	0	0
Symmetry	C1	C1
N Imag	0	0
Rotational Con. (GHz)	-	-
Rotational Con. (GHz)	-	-
Rotational Con. (GHz)	-	-
H298		
H 6-31+g** PCM	-493.954533	-493.954763
H 6-31g*	-493.807603	-493.802423
G298		
G 6-31+g** PCM	-493.999822	-493.999920
G 6-31g*	-493.852892	-493.847580



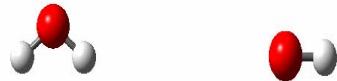
Compound	AMPO-OOH cis-2a	AMPO-OOH trans-2
file	oxam1cis.log	oxam1trans.log
E 6-31+g** PCM	-645.571515	-645.570429
E 6-31g*	-645.5120242	-645.5104792
ZPE (raw)	0.185303	0.18474
Therm Corr to H (raw)	0.198206	0.197989
Therm Corr to G (raw)	0.146749	0.145359
H (raw)	-645.313818	-645.31249
G (raw)	-645.365275	-645.365120
ZPE (scaled)	0.181708	0.181156
Electronic State		
s2 6-31g*	0.753900	0.754100
Symmetry	C01	C01
N Imag	0.000000	0.000000
Rotational Con. (GHz)		
Rotational Con. (GHz)		
Rotational Con. (GHz)		
H298		
H 6-31+g** PCM	-645.376904	-645.376024
H 6-31g*	-645.317413	-645.316074
G298		
G 6-31+g** PCM	-645.428361	-645.428654
G 6-31g*	-645.368870	-645.368704



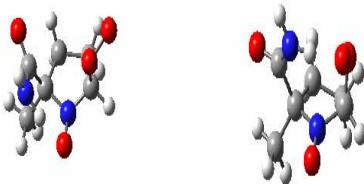
Compound	AMPO-OOH cis-2b	AMPO-OOH cis-3
file	oxam2cis.log	oxam3cis.log
E 6-31+g** PCM	-645.574192	-645.570259
E 6-31g*	-645.5047082	-645.5016459
ZPE (raw)	0.184564	0.184684
Therm Corr to H (raw)	0.197839	0.197844
Therm Corr to G (raw)	0.145802	0.146038
H (raw)	-645.306869	-645.303802
G (raw)	-645.358906	-645.355608
ZPE (scaled)	0.180983	0.181101
Electronic State		
s2 6-31g*	0.753700	0.753400
Symmetry	C01	C01
N Imag	0.000000	0.000000
Rotational Con. (GHz)		
Rotational Con. (GHz)		
Rotational Con. (GHz)		
H298		
H 6-31+g** PCM	-645.379934	-645.375998
H 6-31g*	-645.310450	-645.307385
G298		
G 6-31+g** PCM	-645.431971	-645.427804
G 6-31g*	-645.362487	-645.359191



Compound	AMPO-O2 cis-1a	AMPO-O2 trans-2	AMPO-O2 cis-1b
file	o2am1cis.log	o2am1trans.log	o2am2cis.log
E 6-31+g** PCM	-645.088216	-645.074298	-645.089314
E 6-31g*	-644.9384327	-644.9154458	-644.9416561
ZPE (raw)	0.171004	0.171068	0.171064
Therm Corr to H (raw)	0.183158	0.183533	0.183162
Therm Corr to G (raw)	0.133489	0.133101	0.133831
H (raw)	-644.755275	-644.731913	-644.758494
G (raw)	-644.804944	-644.782345	-644.807825
ZPE (scaled)	0.167687	0.167749	0.167745
Electronic State			
s2 6-31g*	0.7536	0.756	0.7535
Symmetry	C01	C01	C01
N Imag	0	0	0
Rotational Con. (GHz)			
Rotational Con. (GHz)			
Rotational Con. (GHz)			
H298			
H 6-31+g** PCM	-644.908375	-644.894084	-644.909471
H 6-31g*	-644.758592	-644.735232	-644.761813
G298			
G 6-31+g** PCM	-644.958044	-644.944516	-644.958802
G 6-31g*	-644.808261	-644.785664	-644.811144



Compound	H2O	Hydroxide ion	Peroxide
file	h2o.log	hydroxide.log	peroxidepcm_04.log
E 6-31+g** PCM	-76.444739	-75.93692	-151.08056
E 6-31g*	-76.4089533	-75.7207738	-150.886985
ZPE (raw)	0.021165	0.007785	0.012502
Therm Corr to H (raw)	0.024944	0.011089	0.016396
Therm Corr to G (raw)	0.002844	-0.008512	-0.009316
H (raw)	-76.384009	-75.709684	
G (raw)	-76.40611	-75.729285	
ZPE (scaled)	0.020754	0.007634	0.012259
Electronic State	0	0.000000	1-A'
s2 6-31g*			0
Symmetry	CS	C*V	CS
N Imag	0	0	0.000000
Rotational Con. (GHz)	-	-	584.231733
Rotational Con. (GHz)	-	-	25.974080
Rotational Con. (GHz)	-	-	24.8684644
H298			
H 6-31+g** PCM	-76.420206	-75.925982	-151.064407
H 6-31g*	-76.384420	-75.709836	-150.870831
G298			
G 6-31+g** PCM	-76.442306	-75.945583	-151.090119
G 6-31g*	-76.406520	-75.729437	-150.896543

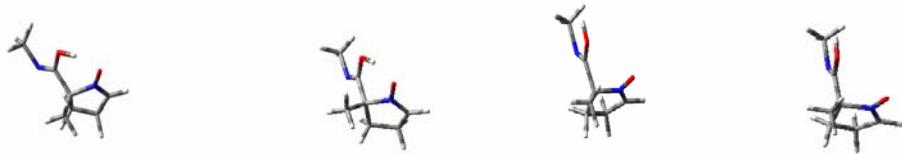


Compound	Restricted AMPO-O2-A	Restricted AMPO-O2-B	OH radical
file	o2amnh2.log	o2amnh2_2.log	hydroxylradical.log
E 6-31+g** PCM	-645.069549	-645.091448	-75.747325
E 6-31g*	-644.9135452	-644.9305319	-75.72345482
ZPE (raw)	0.170302	0.171068	0.008304
Therm Corr to H (raw)	0.182972	0.183533	0.011609
Therm Corr to G (raw)	0.131819	0.132969	-0.008638
H (raw)	-644.730573	-644.746999	
G (raw)	-644.781726	-644.797563	
ZPE (scaled)	0.166998	0.167749	0.008143
Electronic State			
s2 6-31g*	0.762700	0.754600	—
Symmetry	C1	C1	C*V
N Imag	0	0	0.000000
Rotational Con. (GHz)	-	-	0
Rotational Con. (GHz)	-	-	551.7460749
Rotational Con. (GHz)	-	-	551.746075
H298			
H 6-31+g** PCM	-644.889881	-644.911234	-75.735877
H 6-31g*	-644.733877	-644.750318	-75.712007
G298			
G 6-31+g** PCM	-644.941034	-644.961798	-75.756124
G 6-31g*	-644.785030	-644.800882	-75.732254

Table S11. Thermodynamic parameters of imic acids and lactims at the PCM/B3LYP/6-31+G//B3LYP/6-31G* level of theory.**



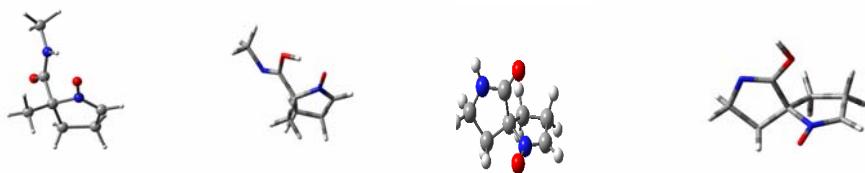
Compound	lactim-1	lactim-2
file	lactim-1.log	lactim-2.log
E 6-31+g**/PCM	-532.682573	-532.692571
E 6-31g*	-532.6271227	-532.6362076
ZPE (raw)	0.172775	0.173227
Therm Corr to H (raw)	0.183099	0.183463
Therm Corr to G (raw)	0.138198	0.138493
H (raw)		
G (raw)		
ZPE (scaled)	0.169423	0.169866
Electronic State	1-A	1-A
s2 6-31g*	0	0
Symmetry	C1	C1
N Imag	0.000000	0.000000
Rotational Con. (GHz)	1.7374065	1.7412608
Rotational Con. (GHz)	1.0386091	1.051746
Rotational Con. (GHz)	0.979379	0.9683941
H298		
6-31+g* */PCM	-532.502826	-532.512469
6-31g*	-532.447376	-532.456105
G298		
6-31+g* */PCM	-532.547727	-532.557439
6-31g*	-532.492277	-532.501075



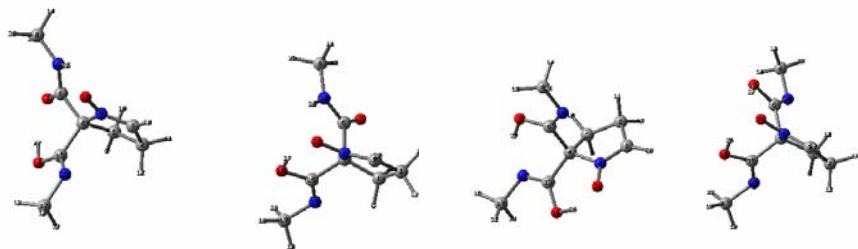
Compound	imic acid-1	imic acid-2	imic-acid-3	imic acid 4
file	mampo-tauto-1.log	mampo-tauto-2.log	mampo-tauto-3.log	mampo-tauto-4.log
E 6-31+g**/PCM	-533.891791	-533.890838	-533.881173	-533.881173
E 6-31g*	-533.8517144	-533.8515979	-533.8347195	-533.8347195
ZPE (raw)	0.1935	0.193587	0.192851	0.192852
Therm Corr to H (raw)	0.205484	0.205599	0.20515	0.20515
Therm Corr to G (raw)	0.156259	0.156097	0.1554	0.155403
H (raw)				
G (raw)				
ZPE (scaled)	0.189746	0.189831	0.189110	0.189111
Electronic State	1-A	1-A	1-A	1-A
s2 6-31g*	0	0	0	0
Symmetry	C1	C1	C1	C1
N Imag	0	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.7733743	1.6443727	1.5167709	1.5167883
Rotational Con. (GHz)	0.8919646	0.9314728	0.991882	0.9918835
Rotational Con. (GHz)	0.751593	0.7960156	0.8340655	0.8340553
H298				
6-31+g* */PCM	-533.690061	-533.688995	-533.679764	-533.679764
6-31g*	-533.649984	-533.649755	-533.633311	-533.633311
G298				
6-31+g* */PCM	-533.739286	-533.738497	-533.729514	-533.729511
6-31g*	-533.699209	-533.699257	-533.683061	-533.683058



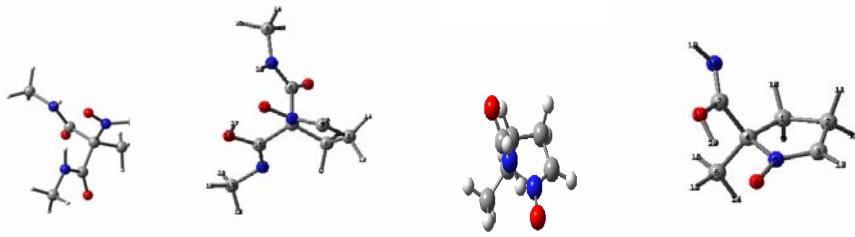
Compound	imic acid-5	imic acid-6	imic-acid-7	imic acid 8
file	mampo-tauto-5.log	mampo-tauto-6.log	mampo-tauto-7.log	mampo-tauto-8.log
E 6-31+g**/PCM	-533.8778057	-533.883821	-533.871604	-533.882671
E 6-31g*	-533.833939	-533.834147	-533.8185907	-533.8295682
ZPE (raw)	0.193689	0.193489	0.192819	0.193459
Therm Corr to H (raw)	0.205588	0.205289	0.205069	0.205437
Therm Corr to G (raw)	0.157528	0.157349	0.156367	0.157178
H (raw)				
G (raw)				
ZPE (scaled)	0.189931	0.189735	0.189078	0.189706
Electronic State	1-A	1-A	1-A	1-A
s2 6-31g*	0	0	0	0
Symmetry	C1	C1	C1	C1
N Imag	0.000000	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.3284142	1.6140638	1.3208873	1.6575612
Rotational Con. (GHz)	1.1383032	1.0209161	1.1376549	0.9351434
Rotational Con. (GHz)	0.9639864	0.7822257	0.9684952	0.8785299
H298				
6-31+g**/PCM	-533.675975	-533.682286	-533.670276	-533.680987
6-31g*	-533.632109	-533.632612	-533.617262	-533.627884
G298				
6-31+g**/PCM	-533.724035	-533.730226	-533.718978	-533.729246
6-31g*	-533.680169	-533.680552	-533.665964	-533.676143



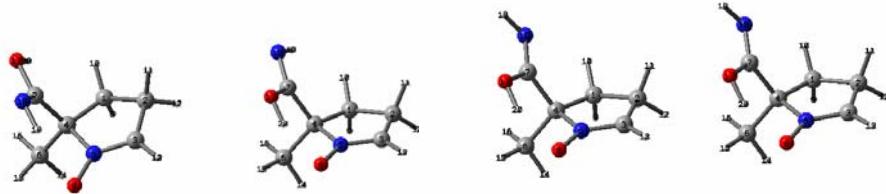
Compound	MAMPO	imic acid-1	TAMPO	lactim-2
file	mampo.log	mampo-tauto-1.log	lam.log	lactim-2.log
E 6-31+g**/PCM	-533.916533	-533.891791	-532.716449	-532.6782205
E 6-31g*	-533.8765506	-533.8517144	-532.6611844	-532.6362076
ZPE (raw)	0.194399	0.1935	0.173838	0.173227
Therm Corr to H (raw)	0.206546	0.205484	0.184087	0.183463
Therm Corr to G (raw)	0.157121	0.156259	0.139172	0.138493
H (raw)			-532.477097	
G (raw)			-532.522013	
ZPE (scaled)	0.190628	0.189746	0.170466	0.169866
Electronic State		1-A		1-A
s2 6-31g*	0	0	0.000000	0
Symmetry	C1	C1	C01	C1
N Imag	0.000000	0	0.000000	0.000000
Rotational Con. (GHz)	1.6022635	1.7733743		1.7412608
Rotational Con. (GHz)	0.9445682	0.8919646		1.051746
Rotational Con. (GHz)	0.8232683	0.751593		0.9683941
H298				
6-31+g**/PCM	-533.713758	-533.690061	-532.535734	-532.498118
6-31g*	-533.673776	-533.649984	-532.480470	-532.456105
G298				
6-31+g**/PCM	-533.763183	-533.739286	-532.580649	-532.543088
6-31g*	-533.723201	-533.699209	-532.525385	-532.501075



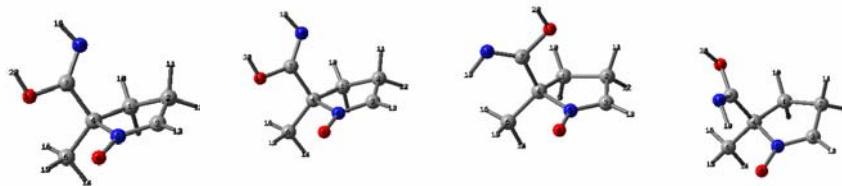
Compound	imic acid-1 diMAPO dimampo-tautomer- 1.log	imic acid-2 diMAPO dimampo-tautomer- 2.log	imic acid-3 diMAPO dimampo-tautomer- 3.log	imic acid-4 diMAPO dimampo-tautomer- 4.log
E 6-31+g**/PCM	-702.592536	-702.594477	-702.569367	-702.566813
E 6-31g*	-702.5412142	-702.5444988	-702.5182755	-702.5169518
ZPE (raw)	0.221006	0.22079	0.219654	0.22007
Therm Corr to H (raw)	0.236187	0.236089	0.234703	0.23521
Therm Corr to G (raw)	0.178437	0.178199	0.177063	0.177792
H (raw)				
G (raw)				
ZPE (scaled)	0.216718	0.216507	0.215393	0.215801
Electronic State	1-A	1-A	1-A	1-A
s2 6-31g*	0	0	0	0
Symmetry	C1	C1	C1	C1
N Imag	0.000000	0.000000	0	0.000000
Rotational Con. (GHz)	0.8983546	0.7780089	0.8713262	0.7547653
Rotational Con. (GHz)	0.6136711	0.651931	0.6435849	0.6571004
Rotational Con. (GHz)	0.509133	0.5351113	0.5068325	0.5333548
H298				
6-31+g**/PCM	-702.360637	-702.362671	-702.338925	-702.335872
6-31g*	-702.309315	-702.312693	-702.287834	-702.286011
G298				
6-31+g**/PCM	-702.418387	-702.420561	-702.396565	-702.393290
6-31g*	-702.367065	-702.370583	-702.345474	-702.343429



Compound	diMAPO	imic acid-2 diMAPO dimampo-tautomer- 2.log	AMPO	imic acid-4 AMPO
file	diAmide_b3lyp_b.log		conh2.log	ampo-taumer-4.log
E 6-31+g**/PCM	-702.62004	-702.594477	-494.613836	-494.590018
E 6-31g*	-702.569436	-702.5444988	-494.5653155	-494.5422652
ZPE (raw)	0.221602	0.22079	0.166017	0.165937
Therm Corr to H (raw)	0.237143	0.236089	0.176458	0.17608
Therm Corr to G (raw)	0.17825	0.178199	0.13143	0.131565
H (raw)			-494.388857	
G (raw)			-494.433885	
ZPE (scaled)	0.217303	0.216507	0.162796	0.162718
Electronic State	1-A	1-A		1-A
s2 6-31g*	0	0	0.000000	0
Symmetry	C1	C1	C01	C1
N Imag	0.000000	0.000000	0.000000	0
Rotational Con. (GHz)	0.7483062	0.7780089	1.755748	1.8000225
Rotational Con. (GHz)	0.6732812	0.651931	1.375520	1.3695707
Rotational Con. (GHz)	0.5456517	0.5351113	1.109713	1.1024017
H298				
6-31+g* */PCM	-702.387196	-702.362671	-494.440599	-494.417157
6-31g*	-702.336592	-702.312693	-494.392078	-494.369404
G298				
6-31+g* */PCM	-702.446089	-702.420561	-494.485627	-494.461672
6-31g*	-702.395485	-702.370583	-494.437106	-494.413919



Compound	imic acid-1 AMPO	imic acid-2 AMPO	imic acid-3 AMPO	imic acid-4 AMPO
file	ampo-taumer-1.log	ampo-taumer-2.log	ampo-taumer-3.log	ampo-taumer-4.log
E 6-31+g**/PCM	-494.578964	-494.586294	-494.590019	-494.590018
E 6-31g*	-494.5195877	-494.5311638	-494.5422657	-494.5422652
ZPE (raw)	0.165187	0.165693	0.165938	0.165937
Therm Corr to H (raw)	0.175824	0.175062	0.176083	0.17608
Therm Corr to G (raw)	0.130454	0.132556	0.131552	0.131565
H (raw)				
G (raw)				
ZPE (scaled)	0.161982	0.162479	0.162719	0.162718
Electronic State	1-A	1-A	1-A	1-A
s2 6-31g*	0	0	0	0
Symmetry	C1	C1	C1	C1
N Imag	0.000000	1 (19.0930i)	0	0
Rotational Con. (GHz)	1.7841839	1.8114619	1.8009574	1.8000225
Rotational Con. (GHz)	1.3122939	1.3467101	1.3689396	1.3695707
Rotational Con. (GHz)	1.1118488	1.0854278	1.1017205	1.1024017
H298				
6-31+g**/PCM	-494.406345	-494.414446	-494.417155	-494.417157
6-31g*	-494.346968	-494.359316	-494.369401	-494.369404
G298				
6-31+g**/PCM	-494.451715	-494.456952	-494.461686	-494.461672
6-31g*	-494.392338	-494.401822	-494.413932	-494.413919



Compound	imic acid-5 AMPO	imic acid-6 AMPO	imic acid-7 AMPO	imic acid-8 AMPO
file	ampo-taumer-5.log	ampo-taumer-6.log	ampo-taumer-7.log	ampo-taumer-8.log
E 6-31+g**/PCM	-494.586736	-494.586735	-494.588553	-494.588311
E 6-31g*	-494.5247616	-494.5247616	-494.5306341	-494.5346322
ZPE (raw)	0.165156	0.165155	0.165822	0.165921
Therm Corr to H (raw)	0.175653	0.175652	0.17615	0.176275
Therm Corr to G (raw)	0.130174	0.130172	0.131374	0.131401
H (raw)				
G (raw)				
ZPE (scaled)	0.161952	0.161951	0.162605	0.162702
Electronic State	1-A	1-A	1-A	1-A
s2 6-31g*	0	0	0	0
Symmetry	C1	C1	C1	C1
N Imag	0.000000	0	0.000000	0.000000
Rotational Con. (GHz)	1.7765613	1.7763588	1.7999383	1.7789832
Rotational Con. (GHz)	1.3664018	1.366602	1.3204954	1.3346348
Rotational Con. (GHz)	1.1317224	1.1317084	1.1642188	1.1071294
H298				
6-31+g**/PCM	-494.414287	-494.414287	-494.415620	-494.415255
6-31g*	-494.352313	-494.352314	-494.357701	-494.361576
G298				
6-31+g**/PCM	-494.459766	-494.459767	-494.460396	-494.460129
6-31g*	-494.397792	-494.397794	-494.402477	-494.406450

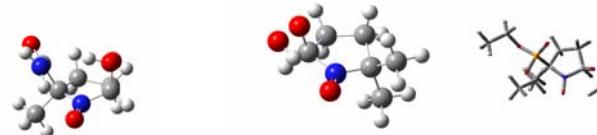
Table S12. Thermodynamic parameters of various hydroperoxyl adducts at the PCM/mPW1K/6-31+G level of theory.**

PCM/mpw1pw91/6-31+g**

ZPE scaling
factor =

0.9515

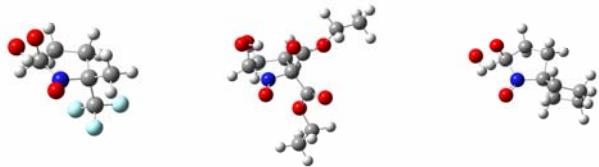
hartree to kcal/mol =



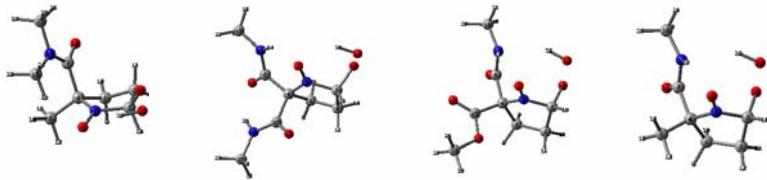
Compound	AMPO-OOH	DMPO-OOH pos	DEPMPO-OOH
file	ampoHO2mpk-neg.log	dmpoHO2mpk-pos.log	DEPMPO-cis-OOH-MW_b.log
E 6-31+g** tight			
PCM	-645.41227	-516.040966	-1201.59037
E 6-31+g**	-645.403074	-516.0416884	-1201.597835
ZPE (raw)	0.186605	0.186691	0.298113
Therm Corr to H (raw)	0.199425	0.19814	0.319079
Therm Corr to G (raw)	0.148501	0.150508	0.247028
H (raw)			
G (raw)			
ZPE (scaled)	0.177555	0.177636	0.283655
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7549	0.755	0.7551
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0
Rotational Con. (GHz)	1.20848	2.12793	0.6519008
Rotational Con. (GHz)	0.94301	1.11279	0.3204499
Rotational Con. (GHz)	0.83032	0.92452	0.2645535
H298			
6-31+g** tight			
PCM	-645.221895	-515.851881	-1201.285749
6-31+g** tight	-645.212633	-515.852603	-1201.293215
G298			
6-31+g** tight			
PCM	-645.272819	-515.899513	-1201.357800
6-31+g** tight	-645.263557	-515.900235	-1201.365266



Compound	CPCOMPO-OOH pos	TAMPO-OOH pos	EMPO-OOH pos
file	tonHO2mpk-pos.log	tamHO2mpk-pos.log	empoHO2mpk-posF.log
E 6-31+g** tight			
PCM	-703.36048	-683.516768	-743.864319
E 6-31+g**	-703.3505219	-683.5025079	-743.867761
ZPE (raw)	0.18237	0.195178	0.230205
Therm Corr to H (raw)	0.194499	0.207434	0.24616
Therm Corr to G (raw)	0.144794	0.157602	0.185749
H (raw)			
G (raw)			
ZPE (scaled)	0.173525	0.185712	0.219040
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7547	0.7549	0.755
Symmetry	C1	C1	C1
N Imag	0.000000	#NAME?	0.000000
Rotational Con. (GHz)	1.4065	1.38883	1.00498
Rotational Con. (GHz)	0.70275	0.72406	0.49482
Rotational Con. (GHz)	0.6488	0.66131	0.42384
H298			
6-31+g** tight			
PCM	-703.174826	-683.318800	-743.629324
6-31+g** tight	-703.164868	-683.304540	-743.632766
G298			
6-31+g** tight			
PCM	-703.224531	-683.368632	-743.689735
6-31+g** tight	-703.214573	-683.354372	-743.693177



Compound	TFMPO-OOH neg	DiEtMPO-OOH pos	CPPO-OOH neg
file	tf_HO2TSmpk-neg.log	DEPO-HO2mpk-posF.log	CPP-OOHmPK-neg.log
E 6-31+g** tight			
PCM	-813.710439	-971.683402	-593.450278
E 6-31+g**	-813.7107885	-971.688757	-593.4484565
ZPE (raw)	0.16371	0.273883	0.224082
Therm Corr to H (raw)	0.177099	0.294016	0.2365
Therm Corr to G (raw)	0.124097	0.224012	0.1853
H (raw)			
G (raw)			
ZPE (scaled)	0.155770	0.260600	0.213214
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7548	0.7547	0.7551
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.47448	0.46707	1.93886
Rotational Con. (GHz)	0.58121	0.37897	0.64222
Rotational Con. (GHz)	0.53542	0.25357	0.58216
H298			
6-31+g** tight			
PCM	-813.541280	-971.402669	-593.224646
6-31+g** tight	-813.541629	-971.408024	-593.222824
G298			
6-31+g** tight			
PCM	-813.594282	-971.472673	-593.275846
6-31+g** tight	-813.594631	-971.478028	-593.274024



Compound	DiMAMPO-OOH pos	DiMAPO-OOH neg	EMAPO-OOH neg	MAMPO-OOH neg
file	DiMAMPO-O2H-MW_pos.log	DiMAPO-O2H-MW_neg.log	EMAPO-O2H-MW_neg.log	MAMPO-O2H-MW_neg_d.log
E 6-31+g** tight				
PCM	-723.99072	-853.368792	-873.209772	-684.70308
E 6-31+g**	-723.9939425	-853.3704894	-873.2121749	-684.7036591
ZPE (raw)	0.242506	0.242248	0.229555	0.214566
Therm Corr to H (raw)	0.258661	0.260372	0.247356	0.229281
Therm Corr to G (raw)	0.199145	0.194637	0.183578	0.173274
H (raw)				
G (raw)				
ZPE (scaled)	0.230744	0.230499	0.218422	0.204160
Electronic State	2-A	2-A	2-A	2-A
s2 6-31g*	0.7551	0.755	0.755	0.755
Symmetry	C1	C1	C1	C1
N Imag	0.000000	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.93755	0.68065	0.69558	1.01416
Rotational Con. (GHz)	0.56359	0.4519	0.5086	0.78766
Rotational Con. (GHz)	0.50521	0.33644	0.38929	0.63776
H298				
6-31+g** tight				
PCM	-723.743821	-853.120169	-872.973549	-684.484205
6-31+g** tight	-723.747043	-853.121866	-872.975952	-684.484785
G298				
6-31+g** tight				
PCM	-723.803337	-853.185904	-873.037327	-684.540212
6-31+g** tight	-723.806559	-853.187601	-873.039730	-684.540792

Compound	water	hydroxide ion
file	H2O_mpW1K.log	hydroxide_mPW1K.log
E 6-31+g** tight		
PCM	-76.421943	-75.908862
E 6-31+g**	-76.41140908	-75.77417583
ZPE (raw)	0.021656	0.008716
Therm Corr to H (raw)	0.025436	0.012021
Therm Corr to G (raw)	0.004022	-0.007537
H (raw)		
G (raw)		
ZPE (scaled)	0.020606	0.008293
Electronic State	1-A1	1-SG
s2 6-31g*	0	0
Symmetry	C2V	C*V
N Imag	0	0
Rotational Con. (GHz)	840.9883957	0
Rotational Con. (GHz)	427.6539316	572.1065075
Rotational Con. (GHz)	283.4936106	572.1065075
H298		
6-31+g** tight		
PCM	-76.397557	-75.897264
6-31+g** tight	-76.387023	-75.762578
G298		
6-31+g** tight		
PCM	-76.418971	-75.916822
6-31+g** tight	-76.408437	-75.782136

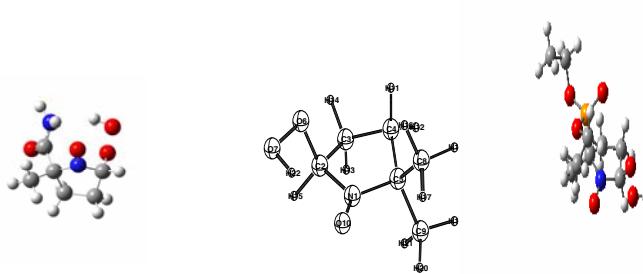
Table S13. Thermodynamic parameters of various hydroperoxyl adducts at the PCM/B3LYP/6-31+G//B3LYP/6-31G* level of theory.**

PCM/b3lyp/6-31+g**//b3lyp/6-31g*

ZPE scaling factor =

0.9806

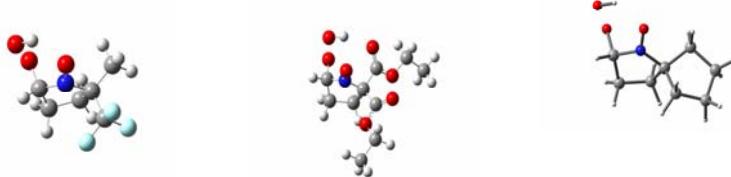
hartree to kcal/mol =



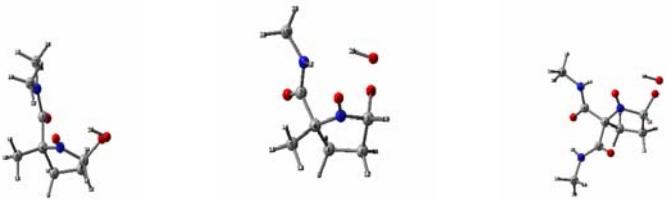
Compound	AMPO-OOH neg	DMPO-OOH C-O pos	DEPMPO-OOH cis-3a
file	disamo-ho2TS_dneg.log	oxdmipoOTS+freq.log	oxdep3cis.log
E 6-31+g** PCM	-645.567811	-516.165541	-1201.802744
E 6-31g*	-645.5074985	-516.1253238	-1201.739257
ZPE (raw)	0.185602	0.18595	0.29634
Therm Corr to H (raw)	0.198308	0.197339	0.317742
Therm Corr to G (raw)	0.147932	0.149905	0.245199
H (raw)		-515.927985	-1201.421514
G (raw)		-515.975419	-1201.494058
ZPE (scaled)	0.182001	0.182343	0.290591
Electronic State	2-A		
s2 6-31g*	0.7544	0.7538	0.753700
Symmetry	C1	C1	C01
N Imag	0.000000		0.000000
Rotational Con. (GHz)	1.1936742	-	
Rotational Con. (GHz)	0.9454383	-	
Rotational Con. (GHz)	0.8284154	-	
H298			
6-31+g** PCM	-645.373104	-515.971809	-1201.490751
6-31g*	-645.312791	-515.931592	-1201.427264
G298			
6-31+g** PCM	-645.423480	-516.019243	-1201.563294
6-31g*	-645.363167	-515.979026	-1201.499807



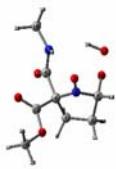
Compound	CPCOMPO-OOH neg	TAMPO-OOH pos	EMPO-OOH pos
file	negtonO2H.log	poslam2.log	posempO2Hdsp.log
E 6-31+g** tight PCM	-703.525957	-683.676389	-744.046421
E 6-31+g**	-703.4702272	-683.6136914	-743.9974642
ZPE (raw)	0.180783	0.193861	0.229199
Therm Corr to H (raw)	0.193052	0.206133	0.245091
Therm Corr to G (raw)	0.143144	0.15639	0.184842
H (raw)			
G (raw)			
ZPE (scaled)	0.177276	0.190100	0.224753
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7543	0.7544	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.346805	1.3703243	1.0129373
Rotational Con. (GHz)	0.726191	0.7182703	0.4838898
Rotational Con. (GHz)	0.640375	0.6558146	0.4174045
H298			
6-31+g** tight PCM	-703.336412	-683.474017	-743.805776
6-31+g** tight	-703.280682	-683.411319	-743.756820
G298			
6-31+g** tight PCM	-703.386320	-683.523760	-743.866025
6-31+g** tight	-703.330590	-683.461062	-743.817069



Compound	TFMPO-OOH neg	DiEtMPO-OOH pos	CPPO-OOH neg
file	tf_HO2TSfneg.log	posDEPO-HO2TSb.log	CPPO2H-b3lyp_neg_d.log
E 6-31+g** tight PCM	-813.900873	-971.922891	-593.586173
E 6-31+g**	-813.8447617	-971.865317	-593.539431
ZPE (raw)	0.162956	0.272421	0.223121
Therm Corr to H (raw)	0.176298	0.292588	0.23547
Therm Corr to G (raw)	0.123448	0.222558	0.184533
H (raw)			
G (raw)			
ZPE (scaled)	0.159795	0.267136	0.218792
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7544	0.7542	0.7539
Symmetry	C1	C1	-
N Imag Rotational Con. (GHz)	0.000000	0.000000	0.000000
Rotational Con. (GHz)	1.4586532	0.4601682	1.9088034
Rotational Con. (GHz)	0.5804589	0.3757929	0.6379774
Rotational Con. (GHz)	0.5331642	0.2520042	0.5749996
H298			
6-31+g** tight PCM	-813.727736	-971.635588	-593.355032
6-31+g** tight	-813.671625	-971.578014	-593.308290
G298			
6-31+g** tight PCM	-813.780586	-971.705618	-593.405969
6-31+g** tight	-813.724475	-971.648044	-593.359227

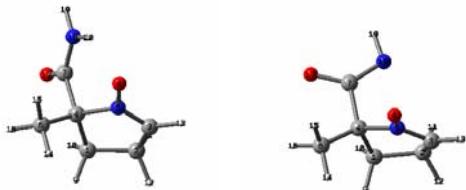


Compound	DiMAMPO-OOH pos file	MAMPO-OOH neg B3LYP_pos.log	DiMAPO-OOH neg DiMAPO-O2H- B3LYP_neg.log
E 6-31+g** tight PCM	-724.165782	-684.868589	-853.575237
E 6-31+g**	-724.1179248	-684.8177671	-853.5154293
ZPE (raw)	0.241901	0.213577	0.240997
Therm Corr to H (raw)	0.257894	0.228158	0.259027
Therm Corr to G (raw)	0.198993	0.173111	0.193964
H (raw)			
G (raw)			
ZPE (scaled)	0.237208	0.209434	0.236322
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.7546	0.7544	0.7545
Symmetry	C1	C1	C1
N Imag	0.000000	0.000000	0.000000
Rotational Con. (GHz)	0.937654	1.00691	0.6725997
Rotational Con. (GHz)	0.5514136	0.7887181	0.4468623
Rotational Con. (GHz)	0.4961908	0.637928	0.3334124
H298			
6-31+g** tight PCM	-723.912581	-684.644574	-853.320885
6-31+g** tight	-723.864724	-684.593752	-853.261078
G298			
6-31+g** tight PCM	-723.971482	-684.699621	-853.385948
6-31+g** tight	-723.923625	-684.648799	-853.326141



Compound	EMAPO-O2H- radical	
file	B3LYP_neg.log	
E 6-31+g** tight PCM	-873.423429	
E 6-31+g**	-873.3674183	
ZPE (raw)	0.228257	
Therm Corr to H (raw)	0.24597	
Therm Corr to G (raw)	0.182879	
H (raw)		
G (raw)		
ZPE (scaled)	0.223829	
Electronic State	2-A	
s2 6-31g*	0.7544	
Symmetry	C1	
N Imag	0.000000	
Rotational Con. (GHz)	0.6971941	
Rotational Con. (GHz)	0.5029197	
Rotational Con. (GHz)	0.3883797	
H298		
6-31+g** tight PCM	-873.181887	
6-31+g** tight	-873.125877	
G298		
6-31+g** tight PCM	-873.244978	
6-31+g** tight	-873.188968	

Table S14. pK_a Calculation for AMPO.

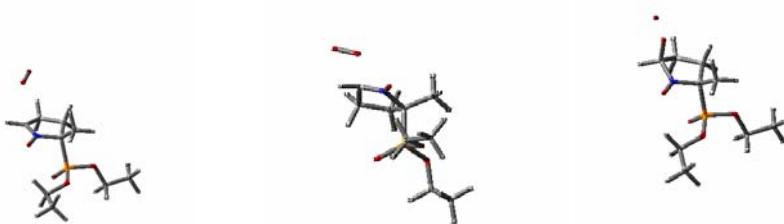


Compound	AMPO	AMPO-NH	Pagas
file	ampo-pka.log	ampo-NH-.log	354.0260421
E 6-311+g* tight (PCM)	-494.733661	-494.2497146	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-494.7006232	-494.1223448	-59.19421109
ZPE (raw)	0.165008	0.150627	
Therm Corr to H (raw)	0.175478	0.160875	
Therm Corr to G (raw)	0.130502	0.116071	
H (raw)			
G (raw)			
ZPE (scaled)	0.161807	0.147705	
Electronic State	1-A	—	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	1.7595215	1.8360258	
Rotational Con. (GHz)	1.3696257	1.301272	
Rotational Con. (GHz)	1.1116692	1.1763246	
H298			
6-311+g* tight (PCM)	-494.561384	-494.091762	
6-311+g*	-494.528346	-493.964392	
G298			
6-311+g* tight (PCM)	-494.606360	-494.136566	
6-311+g*	-494.573322	-494.009196	

Table S15. Thermodynamic parameters of trans superoxide adducts at the PCM/B3LYP/6-31+G//B3LYP/6-31G* and PCM/mPW1K/6-31+G** levels of theory.**



Compound	DEPMPO-O2 pos trans DEPMPO-O2-trans-TS- B3LYP-B_pos.log	DEPMPO-O2 TS trans DEPMPO-O2-trans-TS-B3LYP- B.log	DEPMPO-O2 neg trans DEPMPO-O2-trans-TS- B3LYP-B_neg.log
E 6-31+g** tight PCM	-1201.307665	-1201.292187	-1201.300845
E 6-31g*	-1201.148377	-1201.143837	-1201.150108
ZPE (raw)	0.282277	0.280551	0.281319
Therm Corr to H (raw)	0.303059	0.301296	0.303043
Therm Corr to G (raw)	0.231611	0.229967	0.228665
H (raw)			
G (raw)			
ZPE (scaled)	0.276801	0.275108	0.275861
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.755500	0.757800	0.757400
Symmetry	C1	C1	C1
N Imag	0.000000	1 (420.7943i)	0.000000
Rotational Con. (GHz)	0.622779	0.624050	0.595059
Rotational Con. (GHz)	0.302259	0.297290	0.286805
Rotational Con. (GHz)	0.238292	0.235800	0.225154
H298			
6-31+g** tight PCM	-1201.010082	-1200.996334	-1201.003260
6-31g* tight	-1200.850794	-1200.847984	-1200.852523
G298			
6-31+g** tight PCM	-1201.081530	-1201.067663	-1201.077638
6-31g* tight	-1200.922242	-1200.919313	-1200.926901
E	1.376756	11.089348	5.656371
H	1.721417	10.348722	6.002654
G	12.611217	21.313195	15.053851



Compound	DEPMPO-O2-Trans TS neg	DEPMPO-O2-Trans TS	DEPMPO-O2-Trans TS pos
file	DEPMPO-O2_trans- TS_mpw1k_neg.log	DEPMPO-O2_trans- TS_mpw1k.log	DEPMPO-O2_trans- TS_mpw1k_pos.log
E 6-31+g** tight			
PCM	-1201.082041	-1201.069990	-1201.095592
E 6-31+g**	-1201.010349	-1201.004294	-1201.012198
ZPE (raw)	0.281732	0.281177	0.283139
Therm Corr to H (raw)	0.303701	0.301984	0.303988
Therm Corr to G (raw)	0.228267	0.230380	0.232173
H (raw)			
G (raw)			
ZPE (scaled)	0.268068	0.267540	0.269407
Electronic State	2-A	2-A	2-A
s2 6-31g*	0.757500	0.756100	0.755600
Symmetry	C1	-	C1
N Imag	0.000000	1 (239.8481i)	0.000000
Rotational Con. (GHz)	0.603813	0.629291	0.632373
Rotational Con. (GHz)	0.280549	0.297312	0.301687
Rotational Con. (GHz)	0.221326	0.236125	0.238236
H298			
6-31+g** tight			
PCM	-1200.792004	-1200.781643	-1200.805336
6-31+g** tight	-1200.720312	-1200.715947	-1200.721942
G298			
6-31+g** tight			
PCM	-1200.867438	-1200.853247	-1200.877151
6-31+g** tight	-1200.795746	-1200.787551	-1200.793757
E	3.411769	10.973886	-5.091612
H	3.704706	10.206280	-4.661401
G	12.225657	21.130593	6.130507

Table S16. Calculated relative enthalpies ΔH_{298K} and free energies ΔG_{298K} (kcal/mol) in aqueous phase and other theoretical parameters for the TS structures of the trans $O_2^{\cdot-}$ addition to DEPMPO at the PCM/mPW1K/6-31+G(d,p) and PCM/B3LYP/6-31+G(d,p)//B3LYP/6-31G(d) (in parentheses) levels of theory.

Structure	$\Delta H_{298K,aq}^e$	$\Delta G_{298K,aq}^e$	$C-O_2^{\cdot-}$ Å	$\langle S^2 \rangle$	Imaginary frequency ^g
DEPMPO-O2 trans					
DEPMPO + $O_2^{\cdot-}$	0.0 (0.0)	0.0 (0.0)	∞	a	
DEPMPO--- $O_2^{\cdot-}$	3.7 (6.0)	12.2 (15.1)	2.55 (2.42)	0.76 (0.76)	0
[DEPMPO- $O_2^{\cdot-}$] [‡]	10.2 (10.3)	21.1 (21.3)	1.64 (1.64)	0.76 (0.76)	240 <i>i</i> (421 <i>i</i>)
DEPMPO- $O_2^{\cdot-}$	-4.7 (1.3)	6.1 (12.6)	1.40 (1.44)	0.76 (0.76)	0

Cartesian Coordinates**mPW1K/6-31+g******Nitrones****DMPO**

C	-0.691816	-1.325203	-0.376615
C	-1.937289	-0.495916	-0.011147
C	-1.410728	0.896916	-0.023190
C	0.508716	-0.440671	-0.013147
N	-0.109378	0.942631	-0.027907
C	1.638470	-0.479984	-1.027455
C	1.024262	-0.679241	1.404111
O	0.643160	1.954596	0.010597
H	-0.687087	-1.524268	-1.452001
H	-0.657178	-2.287170	0.139362
H	-2.333486	-0.760164	0.978837
H	-2.755544	-0.641596	-0.722663
H	-1.968451	1.821837	0.024630
H	1.272022	-0.247786	-2.030634
H	2.407496	0.248701	-0.766620
H	2.082417	-1.478944	-1.042349
H	1.537326	-1.643082	1.454387
H	1.727590	0.108086	1.683051
H	0.205566	-0.686208	2.129236

AMPO

C	0.834670	-1.410454	0.459279
C	1.911058	-1.070011	-0.588485
C	1.837876	0.413847	-0.668924
C	-0.076968	-0.183287	0.518573
N	0.787757	0.897929	-0.078788
C	-0.506580	0.220460	1.922671
C	-1.337503	-0.366622	-0.364583
O	0.412789	2.114173	-0.012454
H	1.299623	-1.561436	1.436508
H	0.254276	-2.298383	0.209517
H	1.692175	-1.519556	-1.565530
H	2.904954	-1.420443	-0.296039
H	2.508843	1.091914	-1.178599
H	0.370043	0.340010	2.563908
H	-1.055446	1.162495	1.905134
H	-1.145801	-0.561051	2.338946
O	-1.830875	-1.474915	-0.515911
N	-1.847753	0.769214	-0.875835
H	-2.678090	0.708852	-1.441759
H	-1.361247	1.649945	-0.733978

EMPO

C	-1.036619	-0.575841	-1.504517
C	-1.354338	-1.884195	-0.755038
C	-1.784247	-1.401871	0.583347

C	-0.862410	0.497557	-0.412093
N	-1.507031	-0.146931	0.787409
O	-1.679735	0.545155	1.827435
C	-1.545880	1.817537	-0.706206
C	0.619623	0.724765	-0.094972
O	1.218497	1.735684	-0.374403
O	1.172345	-0.354320	0.466625
C	2.569522	-0.265028	0.813244
C	3.451994	-0.651566	-0.354069
H	-1.878598	-0.289453	-2.139408
H	-0.156481	-0.660415	-2.144357
H	-0.471544	-2.529807	-0.668929
H	-2.130110	-2.467548	-1.260122
H	-2.219633	-1.975740	1.389280
H	-1.464926	2.484503	0.151746
H	-1.073155	2.291886	-1.567161
H	-2.602499	1.643685	-0.921413
H	2.681421	-0.956376	1.649355
H	2.778001	0.751168	1.152046
H	3.336740	0.053287	-1.179663
H	3.215563	-1.658248	-0.707533
H	4.499700	-0.638732	-0.041133

TAMPO

C	0.785041	-0.696626	1.369837
C	2.158524	-0.882810	0.699810
C	2.211261	0.268559	-0.242174
C	-0.023499	0.125210	0.360770
N	1.053850	0.836632	-0.411747
C	-1.083096	1.090616	0.869929
C	-0.786852	-0.792676	-0.617574
O	0.744779	1.810441	-1.153213
H	0.891877	-0.119932	2.293178
H	0.302732	-1.644902	1.614338
H	2.215385	-1.831829	0.154897
H	2.977470	-0.867907	1.424953
H	3.058850	0.631596	-0.805708
H	-0.946187	1.356896	1.919252
H	-1.004319	1.993900	0.257925
O	-0.283680	-1.600452	-1.375056
C	-2.430612	0.395460	0.612383
H	-2.811332	-0.106361	1.510138
H	-3.192838	1.098953	0.268051
N	-2.106849	-0.567185	-0.420266
H	-2.794037	-1.122864	-0.904670

TFMPO

C	0.800026	-1.212004	0.947404
C	1.935681	-1.332524	-0.086129
C	2.061790	0.058344	-0.595002
C	0.055544	0.083163	0.592325
N	1.071257	0.828661	-0.242560
C	-0.356954	0.942929	1.773299
C	-1.159278	-0.216580	-0.300451

O	0.877339	2.042906	-0.515311	H	-3.955576	-1.625615	0.432598
H	1.216265	-1.103727	1.951341	H	-3.585623	-1.756442	-1.280873
H	0.138374	-2.078604	0.956761	H	-4.003461	0.854011	-0.770047
H	1.683524	-2.028860	-0.894903	H	-0.275715	-0.937163	2.361378
H	2.864252	-1.692091	0.366821	H	-0.706404	0.784295	2.266675
H	2.839662	0.471221	-1.221662	H	-1.978483	-0.440314	2.468958
H	0.519356	1.152582	2.389438	H	1.476283	2.338294	-1.392202
H	-0.770115	1.890144	1.427122	H	0.281702	2.903924	-0.205954
H	-1.097122	0.418366	2.380238	H	2.383877	4.270317	-0.071519
F	-0.807366	-0.904206	-1.404499	H	2.134858	3.366882	1.431090
F	-1.810967	0.877283	-0.696384	H	3.328071	2.804083	0.244907
F	-2.040840	-0.985619	0.376057	H	2.589136	-1.598994	-1.336363

CPCOMPO

C	0.745262	-0.826326	1.304315
C	2.122017	-0.979202	0.632259
C	2.211988	0.254337	-0.195864
C	-0.031450	0.104459	0.365508
N	1.068118	0.859433	-0.327961
C	-1.089614	1.024157	0.937782
C	-0.803021	-0.700204	-0.695482
O	0.784399	1.902245	-0.977916
H	0.852014	-0.336082	2.275979
H	0.242226	-1.782657	1.459323
H	2.166301	-1.874413	0.001240
H	2.931354	-1.052251	1.364122
H	3.075165	0.651538	-0.710414
H	-0.959391	1.225906	2.002243
H	-1.033559	1.964813	0.381574
O	-0.332205	-1.402263	-1.546836
C	-2.395559	0.290512	0.633284
H	-2.723193	-0.350947	1.456415
H	-3.213241	0.954691	0.353871
O	-2.123723	-0.552861	-0.497676

DEPMPO

C	-1.793091	-1.659714	-0.008376
C	-3.255271	-1.295196	-0.345436
C	-3.221679	0.187420	-0.433643
C	-1.149111	-0.347905	0.480726
N	-2.110537	0.699050	0.003943
P	0.458627	-0.068101	-0.394685
C	-1.016366	-0.225090	1.994287
O	-1.790050	1.919440	0.112357
O	1.246387	1.148699	0.288695
C	1.271629	2.461554	-0.325992
C	2.345616	3.267838	0.363657
O	0.344846	-0.009118	-1.872384
O	1.242929	-1.335825	0.216583
C	2.577733	-1.624402	-0.242671
C	2.970952	-2.985738	0.279921
H	-1.291306	-2.020806	-0.907843
H	-1.714590	-2.436781	0.752816

H	-3.955576	-1.625615	0.432598
H	-3.585623	-1.756442	-1.280873
H	-4.003461	0.854011	-0.770047
H	-0.275715	-0.937163	2.361378
H	-0.706404	0.784295	2.266675
H	-1.978483	-0.440314	2.468958
H	1.476283	2.338294	-1.392202
H	0.281702	2.903924	-0.205954
H	2.383877	4.270317	-0.071519
H	2.134858	3.366882	1.431090
H	3.328071	2.804083	0.244907
H	2.589136	-1.598994	-1.336363
H	3.248325	-0.845890	0.133753
H	3.986780	-3.226940	-0.044591
H	2.944846	-3.006089	1.371883
H	2.296265	-3.756788	-0.098832

DEPO

C	-0.063413	0.942888	1.565856
C	-0.090944	2.479450	1.458516
C	-0.683083	2.693422	0.110613
C	0.000156	0.482442	0.101804
N	-0.664659	1.617994	-0.624684
O	-1.083797	1.435641	-1.795134
C	1.451303	0.374693	-0.383326
O	1.970718	1.116528	-1.176916
O	2.069580	-0.615055	0.260569
C	3.430824	-0.874286	-0.137745
C	3.917434	-2.063684	0.653378
H	-0.993790	0.583614	2.007575
H	0.773269	0.557950	2.148588
H	0.915789	2.913361	1.525206
H	-0.688057	2.933621	2.254319
H	4.026223	0.022621	0.052632
H	3.440421	-1.063361	-1.213736
H	3.301369	-2.942631	0.452696
H	3.894727	-1.860314	1.726633
H	4.948045	-2.293441	0.371172
C	-0.778544	-0.790715	-0.248085
O	-0.343624	-1.692897	-0.917099
O	-2.003531	-0.745712	0.273409
C	-2.886415	-1.821708	-0.104756
H	-2.928246	-1.857374	-1.195785
H	-2.456055	-2.762101	0.249123
C	-4.235609	-1.542018	0.510321
H	-4.640340	-0.594660	0.147921
H	-4.932568	-2.338919	0.238854
H	-4.172388	-1.500637	1.600283
H	-1.080798	3.605370	-0.310791

CPPO

C	-0.925430	-1.351746	0.597395
C	-2.283635	-1.007286	-0.038141
C	-2.182031	0.470179	-0.202342

C	0.015241	-0.224119	0.164595	O	-1.880391	-1.279187	1.345284
N	-0.959281	0.901968	-0.081901	H	-1.327432	2.290214	-0.187979
C	0.794583	-0.481170	-1.147737	H	0.002498	1.816464	-1.252883
O	-0.524423	2.080378	-0.209032	H	-1.383355	0.253375	-2.455309
H	-0.546562	-2.333278	0.303272	H	-2.630638	1.405440	-1.976320
H	-1.023820	-1.343835	1.687305	H	-1.189924	1.424219	2.106472
H	-3.126864	-1.305027	0.591942	H	-0.150932	0.045447	2.467405
H	-2.423356	-1.503825	-1.008178	H	0.559863	1.573053	1.902636
H	0.381325	-1.320877	-1.713957	O	0.433337	-1.607587	-0.622358
H	0.725359	0.416744	-1.769525	N	1.976931	-0.061493	-0.053147
C	2.247222	-0.678068	-0.710756	C	3.035202	-0.974197	-0.447467
H	2.401796	-1.695962	-0.331400	H	-3.315917	-0.910815	-0.807944
H	2.956208	-0.522755	-1.528388	H	2.660150	-1.994523	-0.412448
H	-2.966695	1.172719	-0.446092	H	3.878525	-0.864555	0.240252
C	1.081355	0.184378	1.201057	H	3.383105	-0.763245	-1.465992
H	0.785594	1.097008	1.722412	C	2.422281	1.292623	0.200358
H	1.170589	-0.617961	1.941642	H	1.598900	2.000806	0.199601
C	2.392843	0.335782	0.425355	H	2.949131	1.367685	1.158798
H	2.461061	1.346379	0.011269	H	3.116106	1.596219	-0.591558
H	3.274826	0.166174	1.048706				

MAMPO

C	1.478301	-1.301498	0.061272
C	2.170757	-0.628897	-1.139210
C	1.851128	0.810724	-0.941690
C	0.441521	-0.289559	0.554482
N	0.937597	1.002758	-0.039539
C	0.360880	-0.160011	2.069825
C	-0.970731	-0.605692	-0.003623
O	0.413408	2.106629	0.325145
H	2.206321	-1.487740	0.854738
H	0.991805	-2.243283	-0.191321
H	1.771934	-0.984026	-2.098141
H	3.248447	-0.814850	-1.158483
H	1.351432	0.043052	2.484410
H	-0.308705	0.651768	2.355973
H	-0.011816	-1.098033	2.486828
O	-1.305516	-1.770711	-0.188169
N	-1.764809	0.462894	-0.196101
C	-3.127672	0.345555	-0.660434
H	2.246466	1.665396	-1.473668
H	-1.356374	1.376929	-0.010194
H	-3.353167	-0.712111	-0.792754
H	-3.260366	0.861586	-1.615613
H	-3.823731	0.770678	0.068172

DiMAMPO

C	-0.851780	1.440573	-0.687084
C	-1.869919	0.721494	-1.589316
C	-2.432686	-0.303701	-0.672196
C	-0.462522	0.392108	0.371245
N	-1.696634	-0.489452	0.384512
C	-0.284742	0.895479	1.797294
C	0.688209	-0.512542	-0.144116

DiMAPO

C	-0.571259	-1.639493	-1.149976
C	-1.407606	-2.529091	-0.211627
C	-1.052483	-2.028606	1.139948
C	-0.125449	-0.449097	-0.296896
N	-0.374977	-0.925408	1.107853
C	1.361913	-0.099300	-0.569797
O	1.795309	-0.228112	-1.705519
C	3.472450	0.710665	0.309810
H	-1.126068	-1.276852	-2.013912
H	0.310255	-2.166201	-1.514978
H	-1.179829	-3.592680	-0.326384
H	-2.485847	-2.417837	-0.381893
H	3.599082	1.353702	-0.562850
H	4.098007	-0.176363	0.168884
C	-0.996045	0.814826	-0.580802
O	-1.505533	0.967188	-1.680201
C	-1.857873	2.911172	0.318839
H	-1.215965	3.742915	0.011444
H	-2.635102	2.782537	-0.434796
H	-1.323777	-2.439680	2.103414
O	0.011666	-0.228649	2.120568
H	-2.317117	3.153818	1.278220
N	-1.107662	1.680976	0.441591
H	-0.684491	1.417239	1.326422
N	2.078245	0.360381	0.468466
H	1.634173	0.335389	1.383690
H	3.804004	1.242488	1.201582

EMAPO

C	-0.457265	1.362354	-1.327949
C	-0.309816	2.697416	-0.567919
C	-0.282456	2.277515	0.857245
C	-0.058326	0.284863	-0.313673

N	-0.161582	0.993902	1.003835	C	0.647545	0.149620	0.381807
C	-1.009325	-0.916313	-0.268939	H	2.497159	0.263509	1.527103
O	-0.673170	-2.061664	-0.432714	H	2.351523	1.504763	0.273471
C	-3.229692	-1.566500	0.074654	H	3.893454	-0.761648	-0.141709
H	0.187008	1.289189	-2.203559	H	2.962069	-0.041193	-1.457477
H	-1.494034	1.219911	-1.632357	H	2.137355	-2.362534	-1.404248
H	-1.134931	3.384599	-0.776641	H	2.028718	-2.317678	0.358618
H	0.615397	3.223085	-0.835047	H	0.387557	-0.670625	-1.625989
H	-2.966821	-2.222996	0.905101	H	-0.275538	-1.709619	-0.375579
H	-3.274320	-2.148041	-0.847324	C	0.061799	-0.243066	1.747332
C	1.390693	-0.225345	-0.546734	H	0.178457	0.575918	2.465972
O	1.868515	-0.192286	-1.672820	H	-0.998726	-0.494010	1.669389
C	3.329727	-1.279972	0.478344	H	0.593035	-1.115322	2.145942
H	3.262808	-2.352842	0.270720	C	-0.131836	1.361753	-0.175605
H	3.899718	-0.810168	-0.323352	O	0.427229	2.444533	-0.408511
H	-0.317658	2.899808	1.740996	N	-1.431451	1.135248	-0.387446
O	-0.080252	0.316044	2.078617	H	-1.961877	1.909830	-0.752587
H	3.846503	-1.131449	1.427344	H	-1.938347	0.206601	-0.190334
O	-2.262904	-0.517360	-0.045117	O	-2.780944	-1.075499	0.077807
N	2.019130	-0.675448	0.547523	O	-3.964883	-0.583554	-0.261738
H	1.492810	-0.673809	1.417122				
H	-4.178053	-1.068442	0.263591				

Superoxide Radical Anion

Miscellaneous

MCCP

C	0.847444	0.111436	-1.205392
C	2.237327	-0.003976	-0.575624
C	1.943599	-0.687547	0.758288
C	0.693845	0.042941	1.253862
C	-0.120797	0.424898	-0.029497
H	0.787118	0.873120	-1.988726
H	0.569707	-0.850295	-1.643167
H	2.670115	0.989392	-0.401547
H	2.938491	-0.558997	-1.205090
H	1.713266	-1.744023	0.587767
H	2.771713	-0.633905	1.471075
H	0.106327	-0.552236	1.957558
H	0.980656	0.965570	1.771398
C	-0.487662	1.911188	-0.007635
H	-1.090844	2.198864	-0.875101
H	-1.021041	2.194211	0.907005
H	0.425762	2.512125	-0.034203
C	-1.330860	-0.512250	-0.101535
O	-1.201983	-1.706506	-0.337189
N	-2.554232	0.019611	0.163329
H	-3.348000	-0.599072	0.136986
H	-2.705157	0.999885	0.315451

MCCP-O₂ complex

C	2.164684	0.452871	0.499479
C	2.878863	-0.504022	-0.466209
C	1.937490	-1.706928	-0.549231
C	0.560472	-1.046656	-0.611058

TS and Displacement Structures

AMPO-O₂ TS

C	-0.311278	-1.072689	-1.329059
C	1.015933	-1.744302	-0.930535
C	1.386049	-1.006646	0.313438
C	-0.881721	-0.468784	-0.023535
N	0.282047	-0.528603	0.893660
C	-2.018512	-1.283917	0.577786
C	-1.342956	0.986437	-0.274301
O	0.193674	-0.055981	2.085359
H	-1.024076	-1.767143	-1.782176
H	-0.103518	-0.274689	-2.043208
H	1.781872	-1.625537	-1.701542
H	0.891275	-2.818450	-0.732132
H	-1.739895	-2.341982	0.619450
H	-2.220499	-0.933346	1.591916
H	-2.918436	-1.157414	-0.025220
O	-2.540927	1.211252	-0.494776
N	-0.383816	1.912551	-0.325314
H	-0.720793	2.842969	-0.519704
H	0.660287	1.793117	-0.082184
H	2.204282	-1.261334	0.972120
O	2.272753	0.443629	-0.546518
O	2.176598	1.575550	0.171121

AMPO-O₂ neg displacement

C	0.261851	-0.534457	-1.348717
C	0.864701	-1.794265	-0.688249
C	0.163811	-1.865740	0.616272
C	-0.901129	-0.078025	-0.442797
N	-0.770508	-0.975369	0.762076
C	-2.279314	-0.311817	-1.038236
C	-0.758393	1.397629	0.013997
O	-1.562704	-0.823037	1.741265
H	-0.107186	-0.737914	-2.357258
H	1.041885	0.229295	-1.411943
H	1.943890	-1.676808	-0.553784
H	0.690397	-2.704978	-1.278804
H	-2.364301	-1.348274	-1.380780
H	-3.048048	-0.109260	-0.292328
H	-2.430941	0.365033	-1.880317
O	-1.663614	2.202798	-0.221833
N	0.390451	1.699280	0.623106
H	0.490456	2.673562	0.862497
H	1.271427	1.081532	0.682827
H	0.345160	-2.557747	1.427358
O	3.153632	0.606423	-0.500488
O	2.662497	0.368594	0.707636

AMPO-O₂ pos displacement

C	-0.357743	-1.069312	-1.314729
C	1.068312	-1.595658	-1.061357
C	1.588417	-0.646760	0.008745
C	-0.841920	-0.467468	0.035263
N	0.402123	-0.458634	0.823821
C	-1.885412	-1.332686	0.728478
C	-1.401450	0.970121	-0.204633
O	0.438610	-0.466129	2.092416
H	-1.036130	-1.856603	-1.654138
H	-0.337161	-0.292199	-2.080271
H	1.692255	-1.582544	-1.958818
H	1.056205	-2.614347	-0.659024
H	-1.560312	-2.378472	0.769583
H	-2.045211	-0.980710	1.749392
H	-2.820096	-1.248391	0.172731
O	-2.574392	1.031728	-0.644500
N	-0.554884	1.954012	0.034720
H	-1.006718	2.830360	-0.216440
H	0.970110	1.848016	0.211576
H	2.385817	-1.007904	0.666577
O	1.976528	0.518030	-0.687036
O	2.002923	1.624586	0.218925

DEPMPO-O₂ TS

C	-1.056585	-1.793607	0.088433
C	-2.569556	-1.663847	0.311994
C	-2.791017	-0.169143	0.294223
C	-0.506942	-0.519235	0.755441
N	-1.603453	0.412290	0.603134
O	-1.497233	1.653811	1.131627
H	-0.837701	-1.787044	-0.982809
H	-0.625200	-2.697618	0.526172
H	-2.858090	-2.053700	1.295949
H	-3.171687	-2.181617	-0.439038
O	-3.254662	0.215946	-1.221221
O	-4.428742	-0.291951	-1.478452
H	-3.658614	0.227153	0.829354
C	-0.141127	-0.693392	2.235279
H	0.803096	-1.227201	2.367477
H	-0.079513	0.298651	2.687775
H	-0.939331	-1.250905	2.737666
P	0.971965	0.074969	-0.202319
O	0.776507	0.317843	-1.657807
O	2.021888	-1.138489	0.115168
O	1.729564	1.266362	0.586579
C	3.238113	-1.184595	-0.628900
H	3.902352	-0.385440	-0.279196
H	3.021349	-1.009360	-1.688061
C	1.258224	2.634191	0.491463
H	1.638654	3.109307	1.400557
H	0.158602	2.617747	0.539835
C	1.799337	3.317379	-0.747375
H	1.421901	2.827357	-1.647149
H	1.472184	4.362981	-0.755703

H	2.894442	3.299047	-0.770182	O	-3.194869	0.464840	-1.076874
C	3.872890	-2.542700	-0.419400	O	-4.459575	-0.143279	-1.436354
H	4.817007	-2.607129	-0.969649	H	-3.697684	0.363810	0.908086
H	4.077127	-2.715998	0.640550	C	-0.239262	-0.872497	2.128878
H	3.209510	-3.335280	-0.774801	H	0.569266	-1.603766	2.186475

DEPMPO-O₂ neg displacement

C	-1.031712	-1.701906	-0.260776	O	0.821133	0.369308	-1.659338
C	-2.535144	-1.393591	-0.400280	O	1.933293	-1.210463	0.107277
C	-2.603666	0.090855	-0.294711	O	1.645610	1.195184	0.665594
C	-0.483068	-0.468104	0.472214	C	3.175366	-1.283961	-0.598642
N	-1.478953	0.582163	0.134999	H	3.826175	-0.469374	-0.260561
O	-1.149311	1.806043	0.386625	H	2.988247	-1.151926	-1.668879
H	-0.573779	-1.787448	-1.250022	C	1.388301	2.580070	0.356295
H	-0.820435	-2.619810	0.292180	H	1.377327	3.089799	1.322378
H	-3.143355	-1.838101	0.393689	H	0.394636	2.685123	-0.082065
H	-2.959067	-1.744603	-1.344245	C	2.465549	3.130929	-0.553714
O	-5.408180	0.334110	-0.824928	H	2.441402	2.620123	-1.518647
O	-5.215243	-0.231203	0.350100	H	2.296614	4.199515	-0.723006
H	-3.468692	0.693608	-0.570388	H	3.457109	3.005928	-0.107921
C	-0.417790	-0.614733	1.990929	C	3.801618	-2.630586	-0.311857
H	0.371794	-1.312201	2.278165	H	4.759278	-2.717734	-0.834038
H	-0.227325	0.357178	2.448668	H	3.978491	-2.756577	0.759371
H	-1.378398	-0.990516	2.355121	H	3.147716	-3.438003	-0.650125
P	1.144379	0.051396	-0.229302				
O	1.172270	0.361113	-1.682500				
O	1.996993	-1.267283	0.195345				
O	1.861163	1.143669	0.716863				
C	3.337559	-1.397037	-0.284117				
H	3.980911	-0.706774	0.273038				
H	3.371049	-1.121117	-1.343297				
C	1.757947	2.555397	0.425272				
H	1.801313	3.041894	1.402886				
H	0.776703	2.754701	-0.009452				
C	2.896763	3.003060	-0.466058				
H	2.828411	2.515656	-1.440910				
H	2.841002	4.086375	-0.615927				
H	3.867186	2.768461	-0.017580				
C	3.776943	-2.830287	-0.081529				
H	4.807705	-2.959225	-0.425499				
H	3.727880	-3.105297	0.975151				
H	3.135558	-3.512373	-0.644736				

DEPMPO-O₂ pos displacement

C	-1.248666	-1.699104	-0.085295
C	-2.735048	-1.511344	0.237772
C	-2.932974	0.002092	0.201627
C	-0.575140	-0.539594	0.670145
N	-1.614830	0.497457	0.623297
O	-1.436912	1.630660	1.181863
H	-1.094440	-1.584772	-1.161252
H	-0.841278	-2.663534	0.228533
H	-2.986468	-1.922010	1.222450
H	-3.415321	-1.920182	-0.515150

O	-3.194869	0.464840	-1.076874
O	-4.459575	-0.143279	-1.436354
H	-3.697684	0.363810	0.908086
C	-0.239262	-0.872497	2.128878
H	0.569266	-1.603766	2.186475
H	0.055355	0.035279	2.658708
H	-1.128816	-1.283831	2.613960
P	0.940553	0.034927	-0.218000
O	0.821133	0.369308	-1.659338
O	1.933293	-1.210463	0.107277
O	1.645610	1.195184	0.665594
C	3.175366	-1.283961	-0.598642
H	3.826175	-0.469374	-0.260561
H	2.988247	-1.151926	-1.668879
C	1.388301	2.580070	0.356295
H	1.377327	3.089799	1.322378
H	0.394636	2.685123	-0.082065
C	2.465549	3.130929	-0.553714
H	2.441402	2.620123	-1.518647
H	2.296614	4.199515	-0.723006
H	3.457109	3.005928	-0.107921
C	3.801618	-2.630586	-0.311857
H	4.759278	-2.717734	-0.834038
H	3.978491	-2.756577	0.759371
H	3.147716	-3.438003	-0.650125

DMPO-O₂ TS

C	-0.462805	-1.521824	-0.571751
C	0.853721	-0.988957	-1.177061
C	0.800787	0.487283	-0.938323
C	-1.071585	-0.343738	0.212092
N	-0.416238	0.811307	-0.443635
C	-0.696415	-0.370698	1.697754
C	-2.580477	-0.221779	0.039521
O	-0.881225	2.018338	-0.272693
O	2.005290	0.751147	0.373944
H	-0.295434	-2.387610	0.076740
H	-1.155775	-1.830454	-1.363003
H	0.947292	-1.229955	-2.241173
H	1.739293	-1.369836	-0.642425
H	1.221864	1.211304	-1.626705
H	0.382412	-0.502139	1.819130
H	-0.980330	0.581769	2.154391
H	-1.224809	-1.183515	2.211938
H	-3.082850	-1.079752	0.499576
H	-2.930447	0.700408	0.508664
H	-2.848359	-0.183372	-1.021103
O	2.636117	-0.350450	0.793252

DMPO-O₂ neg displacement

C	-0.485129	-1.266690	-0.944391
C	0.745691	-0.420154	-1.310490
C	0.306184	0.945134	-0.938547
C	-1.191983	-0.454498	0.148023

N	-0.760314	0.947363	-0.191191	H	-1.625349	2.526789	-0.048864
C	-0.642122	-0.760535	1.541991	H	-0.217109	2.750112	1.004918
C	-2.708369	-0.536252	0.111492	H	-0.071882	3.093225	-0.737744
O	-1.368830	1.942317	0.348871	C	1.378729	0.865798	-0.203175
O	3.023200	0.654651	0.451649	O	1.781852	-0.412666	-0.102190
H	-0.217492	-2.267303	-0.592792	C	3.190891	-0.618759	-0.032460
H	-1.154714	-1.375703	-1.806595	C	3.423488	-2.094761	0.200564
H	1.015422	-0.499549	-2.369588	O	2.162041	1.784322	-0.329798
H	1.641144	-0.702462	-0.707712	H	3.655670	-0.273599	-0.962670
H	0.807180	1.877889	-1.150159	H	3.596532	-0.011650	0.782042
H	0.451379	-0.734997	1.536987	H	4.496184	-2.297617	0.276974
H	-1.008594	-0.016350	2.253826	H	2.940064	-2.415340	1.126023
H	-0.972931	-1.753678	1.864404	H	3.017215	-2.689996	-0.621315
H	-3.030361	-1.552983	0.358249	O	-3.139838	-0.359259	0.400566
H	-3.137898	0.164907	0.830064	O	-3.912576	-1.202524	-0.255107
H	-3.088951	-0.281385	-0.882258	H	-1.593507	-1.735687	1.000835
O	3.079678	-0.663462	0.493910				

EMPO-O₂ neg displacement

DMPO-O₂ pos displacement

C	-0.283405	-1.540417	-0.215126
C	0.860885	-1.101199	-1.140908
C	1.149523	0.364369	-0.795621
C	-1.068756	-0.264293	0.160307
N	-0.200403	0.810483	-0.358767
C	-1.207264	-0.100954	1.673902
C	-2.426613	-0.176330	-0.538911
O	-0.542936	2.031877	-0.291955
O	2.143916	0.569679	0.119534
H	0.159142	-1.966309	0.685309
H	-0.945379	-2.278004	-0.687196
H	0.565880	-1.171180	-2.196362
H	1.762594	-1.690897	-0.970848
H	1.406156	0.982259	-1.667128
H	-0.193411	-0.097486	2.093556
H	-1.711337	0.842027	1.908869
H	-1.790251	-0.929745	2.093254
H	-3.108966	-0.932666	-0.136623
H	-2.863230	0.813954	-0.382764
H	-2.323477	-0.341154	-1.616875
O	1.936380	-0.350460	1.238211

EMPO-O₂ TS

C	-0.731109	0.375586	-1.510408
C	-1.205649	-1.027292	-1.104729
C	-1.502640	-0.859732	0.360107
C	-0.153267	0.984992	-0.212008
N	-0.708044	0.125121	0.820052
C	-0.537614	2.443621	0.007585
O	-0.431599	0.383139	2.093175
H	-1.584008	0.982354	-1.826360
H	-0.005922	0.364314	-2.330629
H	-0.413701	-1.773040	-1.238270
H	-2.093901	-1.356534	-1.651322

C	-0.749388	0.349511	-1.483791
C	-1.217097	-1.060168	-1.105026
C	-1.693981	-0.887810	0.331171
C	-0.170222	0.956613	-0.178711
N	-0.706479	0.056738	0.850521
C	-0.606000	2.395676	0.070505
O	-0.473724	0.261623	2.084263
H	-1.609595	0.951961	-1.785251
H	-0.022249	0.364194	-2.301568
H	-0.401533	-1.787438	-1.165602
H	-2.084272	-1.395816	-1.680276
H	-1.697117	2.425646	0.074546
H	-0.237602	2.740807	1.038625
H	-0.215400	3.053591	-0.708947
C	1.355526	0.875242	-0.201985
O	1.800755	-0.381845	-0.052090
C	3.219206	-0.551882	-0.066680
C	3.503197	-2.013795	0.193014
O	2.100829	1.815246	-0.384715
H	3.610729	-0.224420	-1.035374
H	3.660709	0.091439	0.700008
H	4.583203	-2.188320	0.201110
H	3.093413	-2.319838	1.158134
H	3.056972	-2.642247	-0.581478
O	-2.942787	-0.276245	0.386069
O	-3.855704	-1.173243	-0.301876
H	-1.674293	-1.811332	0.928249

EMPO-O₂ pos displacement

C	-0.754985	0.255622	-1.355836
C	-1.341459	-1.027495	-0.737468
C	-1.234848	-0.767207	0.713171
C	-0.013963	0.979922	-0.208329
N	-0.487314	0.258353	1.005908
C	-0.352200	2.455081	-0.087105
O	-0.132056	0.711505	2.159431

H	-1.569573	0.897159	-1.701084
H	-0.100278	0.061611	-2.209864
H	-0.763038	-1.919495	-1.017070
H	-2.400730	-1.180590	-1.026277
H	-1.435733	2.560594	-0.001958
H	0.114664	2.873319	0.805321
H	0.002134	2.994458	-0.967706
C	1.496608	0.795454	-0.330077
O	1.867113	-0.471949	-0.097344
C	3.268197	-0.742086	-0.177322
C	3.473669	-2.188341	0.210967
O	2.279549	1.659740	-0.662157
H	3.615252	-0.537687	-1.195381
H	3.797101	-0.060287	0.494655
H	4.538226	-2.437359	0.171840
H	3.110363	-2.369018	1.225005
H	2.937181	-2.855327	-0.468253
O	-3.988714	-0.540872	0.474897
O	-4.279473	-0.988626	-0.728681
H	-1.651825	-1.359928	1.512237

CPCOMPO-O₂ TS

C	0.154009	-0.530484	-1.421388
C	1.449692	-1.171415	-0.911535
C	1.654176	-0.493653	0.420772
C	-0.609277	-0.237369	-0.121565
N	0.450928	-0.044264	0.842926
C	-1.600648	-1.306482	0.363494
C	-1.506211	1.000961	-0.286773
O	0.115380	0.134687	2.133567
H	-0.412506	-1.172091	-2.104248
H	0.374673	0.412840	-1.928091
H	2.302000	-1.039953	-1.583339
H	1.316101	-2.248580	-0.745549
H	-1.400024	-2.295632	-0.056379
H	-1.478877	-1.322701	1.453275
O	-1.181231	2.131917	-0.527930
C	-2.967355	-0.768164	-0.031276
H	-3.327859	-1.176392	-0.983557
H	-3.739385	-0.923556	0.726857
H	2.263730	-0.994120	1.175692
O	2.704200	0.777272	0.115375
O	3.864874	0.320959	-0.266015
O	-2.815804	0.648874	-0.195688

CPCOMPO-O₂ neg displacement

C	-0.231293	-1.267007	-0.094198
C	-1.536613	-0.675322	-0.657875
C	-1.307914	0.780121	-0.538160
C	0.787527	-0.122398	-0.199089
N	-0.070528	1.091695	-0.270967
C	1.756777	-0.136298	-1.378548
C	1.722771	-0.071386	1.010437
O	0.490614	2.240740	-0.177512

H	0.108417	-2.164820	-0.618249
H	-0.378020	-1.519434	0.959273
H	-2.460147	-0.989568	-0.116783
H	-1.695160	-0.946400	-1.712015
H	1.385538	-0.712977	-2.228223
H	1.921668	0.901430	-1.681756
O	1.443398	0.132998	2.157623
C	3.026841	-0.719864	-0.771259
H	3.068437	-1.811711	-0.855322
H	3.945427	-0.299845	-1.184911
H	-2.059495	1.547596	-0.650879
O	-4.270100	0.376689	0.170940
O	-4.232507	-0.914923	0.448732
O	2.987150	-0.382156	0.619941

CPCOMPO-O₂ pos displacement

C	0.183058	-0.839970	-1.171304
C	1.448652	-1.358968	-0.485919
C	1.805064	-0.241092	0.493142
C	-0.594919	-0.207924	-0.005950
N	0.477028	0.285118	0.854183
C	-1.538466	-1.163155	0.733631
C	-1.553071	0.892286	-0.477616
O	0.204007	0.801378	1.985004
H	-0.400761	-1.612594	-1.681610
H	0.447457	-0.062096	-1.891750
H	2.313547	-1.460656	-1.148597
H	1.260618	-2.304289	0.037559
H	-1.211180	-2.203826	0.684444
H	-1.580497	-0.846867	1.779992
O	-1.300744	1.987980	-0.891149
C	-2.871582	-0.925381	0.041419
H	-3.013586	-1.579053	-0.826958
H	-3.737688	-1.024181	0.699283
H	2.312173	-0.596422	1.404133
O	2.535200	0.759543	-0.120798
O	3.771270	0.115298	-0.528566
O	-2.834945	0.430723	-0.419515

TAMPO-O₂ TS

C	0.169259	-0.348417	-1.480348
C	1.464915	-1.043884	-1.047845
C	1.660183	-0.538742	0.360759
C	-0.604137	-0.213698	-0.162593
N	0.453684	-0.142622	0.825646
C	-1.585490	-1.351925	0.192027
C	-1.505373	1.038233	-0.188775
O	0.117220	-0.122992	2.127810
H	-0.392104	-0.903311	-2.239707
H	0.388244	0.650930	-1.866444
H	2.321642	-0.826243	-1.691432
H	1.336854	-2.134206	-1.018876
H	-1.383140	-2.271563	-0.363344
H	-1.431065	-1.517349	1.264891

O	-1.164220	2.197138	-0.350187
C	-2.997396	-0.812914	-0.066176
H	-3.403790	-1.160676	-1.027827
H	-3.703907	-1.105124	0.719617
N	-2.797797	0.619735	-0.076856
H	2.262134	-1.134686	1.050488
O	2.713964	0.754697	0.230650
O	3.876533	0.346428	-0.202070
H	-3.545828	1.288350	-0.160808

TAMPO-O₂ neg displacement

C	-0.276180	-1.187200	-0.131831
C	-1.587830	-0.474308	-0.507399
C	-1.274039	0.939454	-0.206909
C	0.792552	-0.086648	-0.174897
N	-0.006561	1.162940	-0.014651
C	1.648431	0.023850	-1.442214
C	1.826298	-0.242705	0.949183
O	0.613997	2.266510	0.174871
H	-0.027428	-2.023757	-0.790986
H	-0.351656	-1.567275	0.890864
H	-2.490015	-0.835804	0.032842
H	-1.833423	-0.575733	-1.574005
H	1.168605	-0.426272	-2.313526
H	1.815352	1.088264	-1.628229
O	1.619380	-0.228944	2.146590
C	2.979567	-0.649460	-1.083401
H	2.989208	-1.710392	-1.369676
H	3.831994	-0.160592	-1.565070
N	3.028281	-0.492578	0.353920
H	-1.983330	1.753718	-0.171090
O	-4.489353	0.221538	-0.179218
O	-4.335872	-0.933406	0.455087
H	3.810640	-0.778174	0.920165

TAMPO-O₂ pos displacement

C	0.187370	-0.695964	-1.267749
C	1.456080	-1.285989	-0.647052
C	1.810932	-0.289394	0.456521
C	-0.592703	-0.199013	-0.042725
N	0.481734	0.203915	0.863959
C	-1.513577	-1.249380	0.605264
C	-1.562982	0.941640	-0.399301
O	0.211213	0.602469	2.041510
H	-0.395220	-1.408699	-1.860852
H	0.446684	0.159140	-1.897154
H	2.321636	-1.313663	-1.315367
H	1.269844	-2.285639	-0.235190
H	-1.174230	-2.271372	0.423805
H	-1.516153	-1.059081	1.682291
O	-1.292532	2.064194	-0.777101
C	-2.902367	-0.972756	0.022191
H	-3.088939	-1.567961	-0.883464
H	-3.704449	-1.185890	0.736517

N	-2.830710	0.440442	-0.278892
H	2.303387	-0.752827	1.326476
O	2.560674	0.765669	-0.026128
O	3.806967	0.155847	-0.463460
H	-3.606833	0.975221	-0.634016

TFMPO-O₂ TS

C	0.254814	-1.295236	0.707358
C	1.266035	-1.400739	-0.443303
C	1.536365	0.043957	-0.757163
C	-0.453579	0.056952	0.488414
N	0.420269	0.740356	-0.460034
C	-0.639821	0.887248	1.757153
C	-1.832300	-0.177885	-0.157169
O	0.227230	2.027067	-0.741968
H	0.785192	-1.253081	1.661752
H	-0.440917	-2.137191	0.748882
H	0.838916	-1.906546	-1.316595
H	2.186072	-1.917027	-0.158019
H	0.331685	0.981537	2.246523
H	-0.975557	1.887052	1.476360
H	-1.353432	0.424208	2.444762
H	2.038646	0.323757	-1.681289
O	2.801633	0.463331	0.326749
O	3.848630	-0.309075	0.144379
F	-1.750345	-0.856000	-1.322568
F	-2.529738	0.938899	-0.401855
F	-2.626752	-0.940850	0.656961

TFMPO-O₂ neg displacement

C	0.420783	-1.226256	0.381183
C	1.327304	-1.000024	-0.841328
C	1.191002	0.453270	-1.066232
C	-0.488640	0.012939	0.469021
N	0.187182	0.994373	-0.431260
C	-0.607343	0.612624	1.862190
C	-1.882061	-0.295717	-0.089070
O	-0.213148	2.219745	-0.442200
H	1.046179	-1.259109	1.275747
H	-0.150630	-2.155372	0.333966
H	0.997212	-1.575621	-1.717571
H	2.377111	-1.254403	-0.604368
H	0.399233	0.810274	2.234752
H	-1.152011	1.556452	1.819307
H	-1.110329	-0.083772	2.537620
H	1.779093	1.071643	-1.726491
O	3.489537	0.507967	0.324426
O	3.989620	-0.707737	0.324119
F	-1.838520	-0.739571	-1.362039
F	-2.732543	0.739462	-0.062428
F	-2.472323	-1.285615	0.637858

TFMPO-O₂ pos displacement

C	0.303572	-1.298690	0.657907
C	1.299568	-1.384370	-0.504094
C	1.693812	0.069700	-0.706983
C	-0.432574	0.046492	0.473328
N	0.413792	0.751006	-0.510006
C	-0.572005	0.863650	1.755491
C	-1.816413	-0.187612	-0.142137
O	0.240877	1.989435	-0.756756
H	0.854297	-1.258019	1.599884
H	-0.387630	-2.143875	0.703692
H	0.841685	-1.802262	-1.405866
H	2.213415	-1.922850	-0.241556
H	0.430787	1.021630	2.155642
H	-1.019643	1.835603	1.541335
H	-1.181034	0.332313	2.491458
H	2.090227	0.302242	-1.705741
O	2.552675	0.511569	0.298958
O	3.726565	-0.332832	0.235750
F	-1.764723	-0.882984	-1.296510
F	-2.490384	0.946017	-0.401955
F	-2.606598	-0.909946	0.699188

DEPO-O₂ TS

C	0.508274	1.324677	1.540534
C	-0.245598	2.510813	0.915430
C	-0.351545	2.173131	-0.562106
C	0.264438	0.187966	0.535545
N	0.173203	0.918407	-0.720372
C	1.438751	-0.788908	0.443469
O	1.391806	-1.966009	0.725007
O	2.564487	-0.170615	0.062051
C	3.679359	-1.020488	-0.198922
C	4.770785	-0.162781	-0.798454
H	0.138906	1.065139	2.533532
H	1.580429	1.526535	1.590119
H	0.273675	3.461183	1.076265
H	-1.251333	2.592437	1.335667
H	3.362985	-1.810346	-0.885804
H	3.999222	-1.498326	0.733658
H	5.077120	0.624572	-0.104400
H	4.417884	0.308037	-1.718466
H	5.645674	-0.777880	-1.030690
C	-1.000471	-0.601572	0.916883
O	-1.505961	-0.579530	2.024248
O	-1.498115	-1.281179	-0.109346
C	-2.770079	-1.891426	0.101564
H	-2.678270	-2.654577	0.882333
H	-3.468856	-1.128018	0.453829
C	-3.203950	-2.481818	-1.221116
H	-2.488875	-3.233694	-1.564532
H	-4.186348	-2.953828	-1.116586
H	-3.264895	-1.698371	-1.979028
H	0.024642	2.878762	-1.310904
O	-1.895059	2.346313	-0.982802
O	-2.697135	1.542812	-0.324653

O 0.273204 0.279702 -1.880674
DEPO-O₂ neg displacement

C	-0.549592	1.625486	-1.194844
C	-0.018059	2.802732	-0.339326
C	0.573641	2.145185	0.908295
C	-0.224467	0.368235	-0.363458
N	-0.227183	0.926842	0.998932
C	-1.260149	-0.737783	-0.464938
O	-1.092304	-1.878572	-0.811505
O	-2.481020	-0.266581	-0.101261
C	-3.521708	-1.238590	-0.058116
C	-4.764953	-0.553873	0.464777
H	-0.034570	1.538216	-2.152203
H	-1.626241	1.710030	-1.357404
H	-0.828060	3.476675	-0.042663
H	0.751109	3.374024	-0.859631
H	-3.211049	-2.063846	0.589649
H	-3.675390	-1.650949	-1.060985
H	-5.065850	0.266679	-0.192152
H	-4.587673	-0.145775	1.462699
H	-5.590939	-1.269352	0.522994
C	1.233893	-0.098312	-0.778374
O	1.410501	-0.386102	-1.988716
O	1.645154	-0.991233	0.230402
C	2.824211	-1.695842	-0.085285
H	2.708575	-2.189516	-1.056895
H	3.666508	-0.994651	-0.167900
C	3.069775	-2.702308	1.021645
H	2.229258	-3.398117	1.097013
H	3.982038	-3.276469	0.823078
H	3.178378	-2.198158	1.986283
H	0.491642	2.702941	1.843567
O	1.927035	1.810924	0.770094
O	2.076715	1.224093	-0.553531
O	-0.357707	0.255072	2.068238

DEPO-O₂ pos displacement

C	-0.418312	1.084740	-1.431389
C	0.554548	2.107954	-0.815388
C	0.387566	1.864592	0.634797
C	-0.463737	-0.023585	-0.364904
N	-0.221685	0.740321	0.893040
C	-1.792630	-0.756066	-0.210248
O	-1.934028	-1.953228	-0.163404
O	-2.808864	0.115472	-0.121759
C	-4.082782	-0.454279	0.190897
C	-5.062036	0.684828	0.356185
H	-0.091190	0.688216	-2.393064
H	-1.417992	1.511892	-1.538004
H	0.306885	3.137168	-1.096072
H	1.615872	1.917217	-1.101321
H	-3.983544	-1.043890	1.106251
H	-4.377105	-1.134592	-0.614284
H	-5.144238	1.268313	-0.564474

H	-4.743242	1.352285	1.159895	H	-2.447208	-1.037819	-0.437996
H	-6.051996	0.290743	0.603686	H	-1.372010	-1.202600	-1.861153
C	0.659858	-1.033096	-0.656117	H	1.617252	-1.209285	-1.777473
O	0.724203	-1.616133	-1.717345	H	2.031668	0.506874	-1.582670
O	1.542172	-1.108941	0.317827	C	3.152425	-0.760378	-0.248016
C	2.781312	-1.779883	0.027597	H	3.150840	-1.812570	0.066946
H	2.577113	-2.850445	-0.079280	H	4.073281	-0.589980	-0.816158
H	3.157431	-1.392615	-0.921611	H	-1.880080	1.435044	-1.158093
C	3.727133	-1.465602	1.161402	O	-3.707044	0.533834	0.640595
H	3.331844	-1.829990	2.113649	O	-4.104317	-0.714054	0.477357
H	4.691553	-1.949018	0.974711	C	1.527393	0.024017	1.334118
H	3.874034	-0.382911	1.217886	H	1.132626	0.912408	1.830778
H	0.733355	2.476040	1.453415	H	1.369911	-0.839200	1.990898
O	3.255548	1.771893	0.475692	C	3.009632	0.151214	0.972686
O	3.434346	1.497763	-0.799817	H	3.224760	1.184981	0.683278
O	-0.547438	0.215890	2.017599	H	3.677639	-0.118192	1.797852

CPPO-O₂ TS

C	0.243228	1.449333	0.405099
C	1.450712	1.335192	-0.534165
C	1.564467	-0.155556	-0.711016
C	-0.640894	0.246989	0.039766
N	0.324552	-0.661233	-0.578569
C	-1.779554	0.565204	-0.968111
O	-0.059711	-1.880493	-0.931534
H	-0.293963	2.400564	0.314126
H	0.587854	1.351034	1.439033
H	2.372270	1.750952	-0.116140
H	1.259566	1.814917	-1.503366
H	-1.601560	1.500500	-1.510289
H	-1.793810	-0.261801	-1.686656
C	-3.071237	0.555595	-0.152633
H	-3.188387	1.498333	0.400603
H	-3.970105	0.422779	-0.766131
H	2.173163	-0.569060	-1.514002
O	2.550257	-0.650000	0.609990
O	3.683240	0.031400	0.635129
C	-1.368141	-0.406795	1.247340
H	-0.873434	-1.347425	1.497431
H	-1.307542	0.261499	2.115249
C	-2.827529	-0.597482	0.825440
H	-2.926340	-1.548284	0.291033
H	-3.526184	-0.607514	1.670093

CPPO-O₂ neg displacement

C	-0.302427	-1.308016	0.061175
C	-1.441584	-0.800112	-0.838556
C	-1.201654	0.662367	-0.830452
C	0.777804	-0.222424	0.007321
N	-0.021282	0.982398	-0.383762
C	1.889442	-0.438787	-1.049504
O	0.523715	2.145698	-0.287317
H	0.090124	-2.287341	-0.231078
H	-0.684844	-1.390206	1.083483

H	-2.447208	-1.037819	-0.437996
H	-1.372010	-1.202600	-1.861153
H	1.617252	-1.209285	-1.777473
H	2.031668	0.506874	-1.582670
C	3.152425	-0.760378	-0.248016
H	3.150840	-1.812570	0.066946
H	4.073281	-0.589980	-0.816158
H	-1.880080	1.435044	-1.158093
O	-3.707044	0.533834	0.640595
O	-4.104317	-0.714054	0.477357
C	1.527393	0.024017	1.334118
H	1.132626	0.912408	1.830778
H	1.369911	-0.839200	1.990898
C	3.009632	0.151214	0.972686
H	3.224760	1.184981	0.683278
H	3.677639	-0.118192	1.797852

CPPO-O₂ pos displacement

C	-0.232207	-1.421256	0.408456
C	-1.441267	-1.318877	-0.524339
C	-1.716481	0.182943	-0.543678
C	0.641428	-0.209531	0.047657
N	-0.356089	0.720865	-0.503243
C	1.728080	-0.514232	-1.016397
O	-0.031184	1.894229	-0.873987
H	0.325556	-2.359901	0.315181
H	-0.578396	-1.329040	1.441744
H	-2.344771	-1.798542	-0.139187
H	-1.209815	-1.689638	-1.530705
H	1.493794	-1.414047	-1.593835
H	1.765199	0.336017	-1.706117
C	3.040249	-0.594792	-0.239556
H	3.122082	-1.559828	0.278415
H	3.925466	-0.488239	-0.876312
H	-2.229560	0.534155	-1.451913
O	-2.387429	0.598391	0.599269
O	-3.673140	-0.083759	0.568711
C	1.427020	0.405384	1.239208
H	0.982164	1.358994	1.529438
H	1.356323	-0.271212	2.098026
C	2.884298	0.535169	0.781791
H	3.030493	1.497848	0.279389
H	3.601406	0.477644	1.607791

MAMPO-O₂ TS

C	0.776578	-0.971964	-1.403946
C	2.167337	-0.387411	-1.093406
C	1.938199	0.303148	0.210175
C	0.064041	-1.101158	-0.036406
N	0.922648	-0.280922	0.851600
C	0.033439	-2.526563	0.499266
C	-1.372647	-0.540076	-0.132899
O	0.603886	-0.108781	2.084969
H	0.820862	-1.937472	-1.915253

H	0.231424	-0.269959	-2.036645
H	2.495635	0.317996	-1.861388
H	2.931538	-1.171969	-0.997209
H	1.030130	-2.974622	0.429725
H	-0.273976	-2.514785	1.546984
H	-0.683159	-3.117106	-0.072854
O	-2.317139	-1.318288	-0.335143
N	-1.502813	0.785799	-0.076606
H	-0.704407	1.469846	0.131793
H	2.707369	0.745588	0.827321
O	1.304042	1.945156	-0.514949
O	0.434479	2.542226	0.318278
C	-2.811543	1.366752	-0.226795
H	-2.706263	2.452394	-0.178286
H	-3.267400	1.090702	-1.184833
H	-3.495162	1.036381	0.564513

MAMPO-O₂ neg displacement

C	-0.344658	-0.977768	-1.296658
C	-0.376223	-2.278387	-0.464263
C	-0.858068	-1.822711	0.861957
C	-1.039328	0.104103	-0.444566
N	-1.215057	-0.574289	0.891145
C	-2.422192	0.490562	-0.943215
C	-0.170593	1.373391	-0.252482
O	-1.707330	0.077983	1.861962
H	-0.859110	-1.090168	-2.254552
H	0.699890	-0.719698	-1.491612
H	0.624868	-2.713719	-0.395473
H	-1.051108	-3.035599	-0.888587
H	-3.023475	-0.409978	-1.105669
H	-2.915875	1.133375	-0.214101
H	-2.329789	1.042412	-1.879740
O	-0.609370	2.480392	-0.584768
N	1.048235	1.165507	0.246627
H	1.470868	0.194453	0.410957
H	-0.939129	-2.402436	1.771277
O	2.796457	-1.307494	-0.669309
O	2.347673	-1.115820	0.563253
C	1.935962	2.285862	0.422883
H	2.877478	1.910540	0.826638
H	2.132929	2.797345	-0.526783
H	1.511363	3.024143	1.112196

MAMPO-O₂ pos displacement

C	-0.767876	1.046828	-1.361296
C	-2.126256	0.354244	-1.138191
C	-1.816697	-0.631167	-0.021033
C	-0.055169	1.053372	0.020891
N	-0.912490	0.147648	0.805134
C	-0.038158	2.431809	0.668001
C	1.396914	0.509877	-0.130637
O	-0.985954	0.161432	2.071878
H	-0.877982	2.063949	-1.746479

H	-0.175162	0.477980	-2.079298
H	-2.498957	-0.148245	-2.034576
H	-2.887997	1.061246	-0.792089
H	-1.035655	2.884896	0.643540
H	0.279921	2.352397	1.709232
H	0.673771	3.054814	0.125227
O	2.257447	1.328375	-0.535761
N	1.557669	-0.773475	0.129954
H	0.447840	-1.795294	0.307846
H	-2.645341	-0.958307	0.615736
O	-1.185394	-1.723085	-0.654857
O	-0.401752	-2.437487	0.306033
C	2.896155	-1.268453	-0.093503
H	2.919218	-2.345240	0.107304
H	3.240803	-1.099857	-1.125285
H	3.635035	-0.780480	0.559495

DiMAMPO-O₂ TS

C	0.243059	-1.962163	-0.950301
C	1.446286	-1.125187	-1.404010
C	1.840558	-0.337668	-0.166316
C	-0.335016	-1.160200	0.231011
N	0.895471	-0.585177	0.773279
C	-0.999961	-2.040800	1.288270
C	-1.448227	-0.215404	-0.332509
O	0.992467	-0.214000	2.059959
H	0.577944	-2.930590	-0.564064
H	-0.495753	-2.131242	-1.734228
H	1.172273	-0.430468	-2.205868
H	2.275280	-1.736255	-1.773809
H	-0.284542	-2.790439	1.636135
H	-1.287286	-1.438385	2.152135
H	-1.877809	-2.532259	0.861343
O	-2.234488	-0.713134	-1.151935
N	-1.585977	1.078176	0.058787
C	-0.789310	1.805103	1.033013
H	2.866778	-0.337417	0.209898
O	1.858414	1.234601	-0.711394
O	2.908736	1.892004	-0.290607
H	-0.148628	1.137715	1.633403
H	-1.477677	2.340755	1.700380
H	-0.150246	2.534792	0.524254
C	-2.610876	1.872857	-0.580744
H	-3.116187	1.272168	-1.335110
H	-3.342783	2.219705	0.160499
H	-2.157923	2.755924	-1.048106

DiMAMPO-O₂ neg displacement

C	-0.372550	-1.456962	-1.421088
C	1.071704	-0.939516	-1.404802
C	1.396460	-0.904037	0.049018
C	-0.925263	-1.054920	-0.040197
N	0.323903	-1.034339	0.777057
C	-1.901021	-2.055858	0.557586

C	-1.640571	0.313167	-0.206127
O	0.222004	-1.055268	2.062918
H	-0.383309	-2.550237	-1.489626
H	-0.985540	-1.061487	-2.232089
H	1.176494	0.067228	-1.823452
H	1.765859	-1.579410	-1.956656
H	-1.435778	-3.044680	0.587290
H	-2.151690	-1.769677	1.580203
H	-2.804604	-2.085979	-0.051700
O	-2.722595	0.266881	-0.805919
N	-1.090407	1.496776	0.158832
C	0.082382	1.735089	1.007218
H	2.395303	-0.799051	0.468929
O	3.075411	1.143705	-0.379133
O	4.031243	0.279550	-0.098532
H	0.138400	0.994742	1.806906
H	-0.048155	2.720582	1.461371
H	1.019916	1.720154	0.438640
C	-1.769617	2.701883	-0.277751
H	-2.495381	2.452057	-1.048900
H	-2.294181	3.180301	0.559362
H	-1.029457	3.406380	-0.669325

DiMAMPO-O₂ pos displacement

C	1.210709	-1.656341	-0.849258
C	1.859439	-0.399372	-1.455692
C	1.686630	0.731921	-0.421968
C	0.277723	-1.133242	0.258273
N	1.062763	0.023178	0.729591
C	0.034501	-2.141064	1.373255
C	-1.097420	-0.763238	-0.365852
O	1.514242	0.085217	1.916572
H	1.967235	-2.286751	-0.368582
H	0.660559	-2.252435	-1.578170
H	1.346150	-0.087861	-2.368813
H	2.913915	-0.561631	-1.695341
H	0.984720	-2.447915	1.814765
H	-0.581379	-1.715409	2.168275
H	-0.476638	-3.012230	0.955617
O	-1.504258	-1.452159	-1.309556
N	-1.843485	0.219933	0.184360
C	-1.410514	1.133858	1.244499
H	2.604072	1.186632	-0.025553
O	0.859897	1.673319	-0.977444
O	0.759877	2.804998	-0.067554
H	-0.937890	0.588845	2.062297
H	-2.313924	1.609764	1.639154
H	-0.703531	1.899574	0.858956
C	-3.053333	0.615509	-0.503901
H	-3.250910	-0.087854	-1.310498
H	-3.899009	0.622242	0.194239
H	-2.932789	1.624065	-0.916285

DiMAPO-O₂ TS

C	0.072571	-0.781312	-1.557456
C	0.655355	-2.147988	-1.160530
C	1.095380	-1.904552	0.238734
C	-0.359425	-0.119509	-0.225608
N	0.428975	-0.891434	0.775774
C	0.041346	1.387124	-0.202698
O	0.433958	-0.549067	1.996926
H	-0.763012	-0.863247	-2.255563
H	0.857933	-0.168352	-2.000789
H	1.493350	-2.436891	-1.800761
H	-0.107541	-2.934514	-1.187937
O	-0.856556	2.269399	-0.353786
N	1.328078	1.608985	-0.113098
H	2.422225	0.659971	0.308304
H	1.544471	-2.618561	0.912372
O	2.920655	-1.077373	-0.239603
O	3.153292	-0.050845	0.605288
C	1.713791	3.001176	-0.163414
H	2.802763	3.071926	-0.077719
H	1.406072	3.482734	-1.102517
H	1.261325	3.586549	0.649126
C	-1.842340	-0.480860	0.043294
O	-2.170450	-1.661607	0.182749
N	-2.704888	0.539592	0.041426
H	-2.253456	1.467328	-0.094805
C	-4.112173	0.327360	0.244014
H	-4.510512	-0.394760	-0.476671
H	-4.319920	-0.063711	1.246522
H	-4.633077	1.278839	0.121106

DiMAPO-O₂ neg displacement

C	0.357447	-1.040808	-1.162208
C	0.817828	-2.308696	-0.412948
C	0.571705	-1.974091	1.008602
C	-0.396026	-0.185855	-0.120015
N	-0.070490	-0.861484	1.184644
C	0.136576	1.270599	-0.028669
O	-0.465553	-0.328572	2.266432
H	-0.298973	-1.285379	-1.997741
H	1.235029	-0.509046	-1.536789
H	1.877450	-2.506638	-0.598328
H	0.234154	-3.190143	-0.705817
O	-0.615872	2.263744	-0.119886
N	1.445417	1.372366	0.133260
H	2.150570	0.533975	0.153083
H	0.848893	-2.548001	1.881917
O	3.546081	-0.444308	-1.231345
O	3.301216	-0.421892	0.070017
C	2.035913	2.684331	0.232979
H	3.111652	2.558114	0.361152
H	1.848895	3.276170	-0.669898
H	1.627075	3.239927	1.083893
C	-1.923283	-0.385415	-0.294448
O	-2.366210	-1.529785	-0.394095
N	-2.680745	0.714359	-0.355354

H -2.166853 1.598249 -0.236390
C -4.110182 0.627430 -0.491815
H -4.377031 -0.062960 -1.296814
H -4.582461 0.261708 0.427325
H -4.504838 1.618873 -0.721291

DiMAPO-O₂ pos displacement

C 0.057178 -0.785430 -1.570173
C 0.779219 -2.089009 -1.185661
C 1.512810 -1.685527 0.081279
C -0.333262 -0.125433 -0.214626
N 0.532740 -0.837229 0.728437
C 0.001484 1.397397 -0.231304
O 0.397353 -0.758385 1.983841
H -0.820688 -0.964434 -2.193922
H 0.740017 -0.122571 -2.104071
H 1.466161 -2.433979 -1.962721
H 0.057997 -2.875212 -0.950793
O -0.896046 2.207765 -0.621160
N 1.234387 1.691365 0.092221
H 2.403980 0.672039 0.516485
H 1.790621 -2.474001 0.786864
O 2.653361 -0.968558 -0.367793
O 3.099493 -0.081707 0.660081
C 1.570382 3.093381 -0.011318
H 2.624727 3.229261 0.250623
H 1.410128 3.488192 -1.025310
H 0.963540 3.716076 0.661639
C -1.796877 -0.525083 0.098512
O -2.092584 -1.706888 0.285883
N -2.687893 0.474234 0.080077
H -2.286215 1.389474 -0.198285
C -4.091237 0.227470 0.269426
H -4.537846 -0.294477 -0.586784
H -4.254318 -0.395563 1.153229
H -4.603542 1.182195 0.404265

EMAPO-O₂ TS

C -0.086222 -0.845150 -1.444093
C 0.470323 -2.223152 -1.055972
C 1.135652 -1.912794 0.241398
C -0.359610 -0.143524 -0.094506
N 0.505574 -0.896296 0.843331
C 0.020327 1.362317 -0.111033
O 0.746339 -0.454833 2.019514
H -0.977713 -0.883572 -2.069301
H 0.697470 -0.291794 -1.961865
H 1.190887 -2.589424 -1.791359
H -0.323560 -2.975287 -0.939210
O -0.865954 2.223403 -0.068621
N 1.324899 1.604398 -0.228065
H 2.095696 0.850400 -0.055991
H 1.637302 -2.620696 0.884848
O 2.753471 -1.197423 -0.517146

O 3.202294 -0.152771 0.198924
C 1.768619 2.975690 -0.226252
H 2.855523 2.980763 -0.330941
H 1.324214 3.539838 -1.053617
H 1.496709 3.490082 0.703601
C -1.820697 -0.256795 0.345918
O -2.219353 -0.555901 1.443778
C -4.027278 0.088937 -0.332970
H -4.555947 0.313428 -1.259046
H -4.383288 -0.852210 0.093384
H -4.181152 0.888564 0.395011
O -2.653814 0.002527 -0.683612

EMAPO-O₂ neg displacement

C 0.210987 -0.983026 -1.129629
C 0.614167 -2.350241 -0.542999
C 0.580148 -2.113109 0.919990
C -0.390555 -0.192424 0.050100
N 0.062040 -0.968091 1.256953
C 0.097079 1.272786 0.206187
O -0.081021 -0.478097 2.410627
H -0.505912 -1.066772 -1.946876
H 1.109393 -0.488324 -1.511014
H 1.618349 -2.625292 -0.879707
H -0.074971 -3.156568 -0.832900
O -0.718552 2.177583 0.399998
N 1.416079 1.427730 0.121514
H 2.111070 0.616586 -0.020568
H 0.952334 -2.755774 1.705317
O 3.273671 -0.534266 -1.608769
O 3.268853 -0.399030 -0.290993
C 1.979054 2.739588 0.316301
H 3.062551 2.660399 0.216072
H 1.600230 3.450067 -0.426912
H 1.732546 3.136406 1.307664
C -1.915237 -0.209243 0.010932
O -2.651940 -0.722784 0.816775
C -3.762713 0.507662 -1.222548
H -3.942723 0.998599 -2.178172
H -4.252359 -0.468916 -1.194456
H -4.144161 1.120830 -0.403259
O -2.352356 0.372759 -1.119445

EMAPO-O₂ pos displacement

C -0.121753 -0.847247 -1.463937
C 0.561491 -2.180813 -1.114833
C 1.435648 -1.777315 0.058282
C -0.343305 -0.130778 -0.107438
N 0.551175 -0.884763 0.785504
C 0.033478 1.391291 -0.194696
O 0.696912 -0.646383 2.019774
H -1.054899 -0.972583 -2.009701
H 0.559127 -0.241415 -2.062933
H 1.151094 -2.578922 -1.943863

H	-0.161523	-2.939600	-0.796622	N	0.322535	-0.464389	0.873549
O	-0.906125	2.188010	-0.415076	C	-2.015579	-1.219158	0.770865
N	1.320718	1.628893	-0.077542	C	-1.366266	0.986987	-0.300904
H	2.439662	0.594510	0.251484	O	0.347808	0.140395	2.028781
H	1.763278	-2.557068	0.753300	H	-1.176185	-1.908528	-1.598975
O	2.543606	-1.120960	-0.537242	H	-0.284418	-0.455703	-2.069733
O	3.122103	-0.194018	0.382388	H	1.641324	-1.792772	-1.718371
C	1.689513	3.018610	-0.220680	H	0.800607	-2.892514	-0.614479
H	2.776801	3.112454	-0.127786	H	-1.708870	-2.258705	0.924094
H	1.388006	3.434596	-1.193900	H	-2.211961	-0.763323	1.745110
H	1.221205	3.654388	0.545012	H	-2.935385	-1.200352	0.183842
C	-1.782303	-0.203252	0.402652	O	-2.567755	1.207671	-0.545824
O	-2.126495	-0.228369	1.558776	N	-0.418258	1.929977	-0.382489
C	-4.027571	-0.069412	-0.216706	H	-0.724317	2.864483	-0.649360
H	-4.610519	-0.089741	-1.137537	H	0.587761	1.793436	-0.149022
H	-4.339243	-0.875610	0.452163	H	2.213219	-1.308334	0.926167
H	-4.158400	0.886806	0.294678	O	2.295000	0.378761	-0.622099
O	-2.673630	-0.228685	-0.613106	O	2.305302	1.541174	0.118307

PCM-B3LYP/6-31+G**

Superoxide

O	0.000000	0.000000	0.673982
O	0.000000	0.000000	-0.673982

AMPO

C	0.767484	-1.483248	0.360348
C	1.876517	-1.122900	-0.657379
C	1.875293	0.368699	-0.639996
C	-0.092916	-0.210433	0.502153
N	0.845249	0.863836	-0.022490
C	-0.500863	0.107977	1.944709
C	-1.373646	-0.267390	-0.377943
O	0.540348	2.119766	0.127052
H	1.216101	-1.720316	1.329814
H	0.158155	-2.332413	0.048958
H	1.654362	-1.489156	-1.670369
H	2.853267	-1.533400	-0.378767
H	2.599958	1.039519	-1.097138
H	0.388035	0.165691	2.580080
H	-1.040445	1.055803	2.004310
H	-1.145057	-0.693546	2.317349
O	-1.999316	-1.331843	-0.477341
N	-1.766176	0.880441	-0.952847
H	-2.629299	0.893203	-1.495103
H	-1.248052	1.745058	-0.800824

AMPO-O₂ TS

C	-0.433442	-1.179554	-1.264922
C	0.920134	-1.838097	-0.897174
C	1.378286	-1.040406	0.286314
C	-0.912224	-0.456574	0.030820

DMPO

C	-0.658074	-1.357415	-0.355267
C	-1.932831	-0.548597	-0.010952
C	-1.440855	0.861952	-0.021226
C	0.529277	-0.429666	-0.010138
N	-0.143627	0.941562	-0.030232
C	1.648739	-0.459747	-1.047975
C	1.071180	-0.651429	1.408702
O	0.580621	2.015213	0.005506
H	-0.647041	-1.586355	-1.426146
H	-0.599683	-2.303220	0.190256
H	-2.337089	-0.804768	0.979360
H	-2.741407	-0.708224	-0.732903
H	-2.036865	1.770901	0.018981
H	1.265650	-0.226269	-2.046608
H	2.434883	0.257049	-0.797655
H	2.085773	-1.463299	-1.073782
H	1.590231	-1.614007	1.453772
H	1.779369	0.137843	1.676851
H	0.261981	-0.662882	2.146592

DMPO-O₂

C	0.872373	1.548354	-0.262864
C	-0.665425	1.581317	-0.263119
C	-1.086056	0.203424	-0.779509
C	1.257732	0.103355	0.133216
N	0.063320	-0.652677	-0.345638
C	1.390982	-0.073019	1.656700
C	2.518715	-0.394900	-0.580408
O	0.043196	-1.928950	-0.442661
O	-2.328487	-0.282693	-0.389546
H	1.311551	2.281304	0.421354
H	1.256044	1.762676	-1.268144
H	-1.070457	2.383874	-0.886373
H	-1.066969	1.682836	0.748713

H	-1.123861	0.163907	-1.882535
H	0.502374	0.299374	2.174371
H	1.515180	-1.131793	1.905697
H	2.267915	0.474000	2.019642
H	3.375479	0.219277	-0.283048
H	2.731400	-1.435222	-0.316902
H	2.407124	-0.327319	-1.667525
O	-2.499577	-0.240276	1.085972

B3LYP/6-31g***Nitrones****DMPO**

C	-0.706387	-1.340149	-0.348268
C	-1.955219	-0.486071	-0.006632
C	-1.414651	0.907153	-0.024821
C	0.509498	-0.451447	-0.012391
N	-0.106807	0.948140	-0.027280
C	1.625228	-0.491793	-1.053304
C	1.057874	-0.672538	1.402803
O	0.654866	1.958242	0.008979
H	-0.705068	-1.577644	-1.417286
H	-0.683045	-2.286502	0.200049
H	-2.370380	-0.742692	0.980166
H	-2.766146	-0.634560	-0.729883
H	-1.967398	1.836770	0.017860
H	1.231540	-0.301752	-2.057634
H	2.375136	0.270582	-0.828892
H	2.102995	-1.477559	-1.050541
H	1.593550	-1.626434	1.455333
H	1.748255	0.135533	1.661204
H	0.251225	-0.689588	2.144425

AMPO

C	0.862856	-1.398142	0.481341
C	1.959760	-1.045194	-0.556633
C	1.842956	0.439040	-0.678868
C	-0.076082	-0.181241	0.521765
N	0.770973	0.915704	-0.109784
C	-0.500428	0.256615	1.925178
C	-1.343435	-0.406812	-0.357521
O	0.370038	2.130091	-0.073989
H	1.315074	-1.544981	1.466899
H	0.299713	-2.295124	0.220648
H	1.780841	-1.532089	-1.526235
H	2.958319	-1.358146	-0.229847
H	2.502095	1.120964	-1.201319
H	0.377797	0.374952	2.568602
H	-1.036113	1.207210	1.886223
H	-1.153922	-0.506284	2.359640
O	-1.784480	-1.533532	-0.544545
N	-1.920290	0.729270	-0.815504
H	-2.725524	0.643883	-1.420016
H	-1.431295	1.616739	-0.710883

EMPO

C	-1.021735	-0.663681	-1.485600
C	-1.402910	-1.921583	-0.661478
C	-1.844881	-1.346264	0.642421
C	-0.848182	0.478322	-0.454931
N	-1.537320	-0.083129	0.782347

O	-1.709236	0.677120	1.777852
C	-1.504962	1.798933	-0.832219
C	0.629620	0.705567	-0.090406
O	1.224439	1.743290	-0.272370
O	1.181566	-0.414560	0.415375
C	2.573513	-0.331789	0.817269
C	3.505557	-0.592449	-0.355672
H	-1.834617	-0.398329	-2.168226
H	-0.122663	-0.817916	-2.087546
H	-0.541500	-2.590277	-0.524657
H	-2.187954	-2.509112	-1.152536
H	-2.309243	-1.861750	1.472974
H	-1.460578	2.488953	0.012027
H	-0.983757	2.246655	-1.681970
H	-2.552834	1.630062	-1.099764
H	2.673344	-1.097161	1.590275
H	2.749585	0.653029	1.255692
H	3.403911	0.191230	-1.111701
H	3.292472	-1.562824	-0.816544
H	4.544814	-0.599790	-0.007607

TAMPO

C	0.818434	-0.692598	1.377970
C	2.190524	-0.862060	0.679396
C	2.213370	0.295431	-0.266155
C	-0.024823	0.115945	0.377028
N	1.041390	0.852000	-0.421652
C	-1.093751	1.078876	0.893335
C	-0.782366	-0.814378	-0.604209
O	0.706723	1.823719	-1.160268
H	0.934030	-0.113438	2.300760
H	0.356244	-1.649913	1.633959
H	2.245494	-1.814168	0.135851
H	3.022673	-0.841468	1.392893
H	3.049317	0.670998	-0.841167
H	-0.973693	1.322680	1.952219
H	-1.000470	1.994672	0.301170
O	-0.272100	-1.637055	-1.344037
C	-2.450074	0.394635	0.600292
H	-2.857180	-0.107179	1.489255
H	-3.200844	1.107550	0.243459
N	-2.110710	-0.570148	-0.434893
H	-2.795199	-1.131111	-0.924091

TFMPO

C	0.805346	-1.214706	0.960778
C	1.944614	-1.328416	-0.083806
C	2.068319	0.071833	-0.587151
C	0.047002	0.078849	0.602265
N	1.069057	0.841413	-0.234334
C	-0.386126	0.943313	1.780753
C	-1.155253	-0.226194	-0.307873
O	0.859893	2.055767	-0.512717
H	1.226464	-1.104669	1.964352

H	0.147459	-2.086290	0.971883	H	-1.916082	-0.481825	2.484682
H	1.684000	-2.023176	-0.894221	H	1.612643	2.387697	-1.399727
H	2.875084	-1.696031	0.364160	H	0.188128	2.835692	-0.430762
H	2.845223	0.488659	-1.214418	H	2.114743	4.402652	0.021189
H	0.470293	1.131666	2.434485	H	1.688844	3.484191	1.479982
H	-0.767432	1.900290	1.420509	H	3.115943	3.024275	0.526113
H	-1.162798	0.432204	2.356599	H	2.705798	-1.539295	-1.329864
F	-0.779066	-0.915237	-1.408766	H	3.282733	-0.715213	0.138104
F	-1.798053	0.876411	-0.712929	H	4.160434	-3.066830	0.040945
F	-2.047798	-0.997480	0.360464	H	3.065705	-2.867660	1.426123
				H	2.497889	-3.688328	-0.044042

CPCOMPO

C	0.786244	-0.814739	1.317981
C	2.163184	-0.943893	0.619742
C	2.214292	0.289112	-0.223357
C	-0.031917	0.093952	0.382337
N	1.051864	0.873903	-0.345961
C	-1.098448	1.014051	0.957242
C	-0.799494	-0.730849	-0.674971
O	0.734852	1.905965	-1.004336
H	0.898858	-0.317975	2.287526
H	0.308345	-1.783522	1.487198
H	2.212279	-1.847611	-0.002107
H	2.986628	-0.997548	1.340997
H	3.062300	0.698927	-0.755531
H	-0.984509	1.197660	2.028902
H	-1.023685	1.963476	0.416777
O	-0.320734	-1.459130	-1.503701
C	-2.416157	0.298020	0.618688
H	-2.777825	-0.332779	1.438219
H	-3.216133	0.976920	0.316601
O	-2.131058	-0.560433	-0.507316

DEPMPO

C	-1.751150	-1.726586	0.010229
C	-3.244381	-1.403786	-0.270931
C	-3.249334	0.082544	-0.397022
C	-1.124132	-0.387112	0.469079
N	-2.134010	0.636151	-0.004438
P	0.470989	-0.073089	-0.437068
C	-0.972183	-0.232624	1.985652
O	-1.847138	1.871874	0.073991
O	1.230102	1.173713	0.246256
C	1.222095	2.490181	-0.382942
C	2.089287	3.400734	0.464581
O	0.338321	-0.026251	-1.915939
O	1.298534	-1.318849	0.185983
C	2.667239	-1.541085	-0.235186
C	3.122391	-2.872173	0.332833
H	-1.277651	-2.076171	-0.910369
H	-1.620821	-2.501684	0.768893
H	-3.899768	-1.735202	0.548398
H	-3.605765	-1.901562	-1.178526
H	-4.060185	0.722680	-0.719531
H	-0.191807	-0.902241	2.355596
H	-0.705090	0.797647	2.229809

H	-1.916082	-0.481825	2.484682
H	1.612643	2.387697	-1.399727
H	0.188128	2.835692	-0.430762
H	2.114743	4.402652	0.021189
H	1.688844	3.484191	1.479982
H	3.115943	3.024275	0.526113
H	2.705798	-1.539295	-1.329864
H	3.282733	-0.715213	0.138104
H	4.160434	-3.066830	0.040945
H	3.065705	-2.867660	1.426123
H	2.497889	-3.688328	-0.044042

DEPO

C	-0.063468	0.942964	1.577203
C	-0.118876	2.489456	1.479621
C	-0.702062	2.706346	0.121555
C	0.002124	0.485516	0.104645
N	-0.667714	1.632554	-0.626957
O	-1.073187	1.452750	-1.806510
C	1.454461	0.373886	-0.395100
O	1.966820	1.097565	-1.213171
O	2.083421	-0.608827	0.269876
C	3.448837	-0.876129	-0.139267
C	3.944625	-2.052684	0.678405
H	-0.983952	0.563949	2.025826
H	0.784899	0.571795	2.154843
H	0.881847	2.939004	1.568020
H	-0.732467	2.926085	2.276153
H	4.046363	0.026222	0.025474
H	3.449764	-1.088563	-1.212283
H	3.323357	-2.936281	0.503026
H	3.927734	-1.823286	1.748925
H	4.975200	-2.291702	0.394311
C	-0.778298	-0.790278	-0.255977
O	-0.340563	-1.689882	-0.932058
O	-2.012620	-0.750245	0.267292
C	-2.893855	-1.838351	-0.112638
H	-2.944295	-1.870367	-1.204755
H	-2.453081	-2.778790	0.232750
C	-4.245705	-1.569622	0.518722
H	-4.659642	-0.620797	0.163698
H	-4.942670	-2.371542	0.252295
H	-4.169578	-1.529257	1.610249
H	-1.107150	3.618134	-0.296279

CPPO

C	-0.543879	-1.448386	-0.400858
C	-2.026462	-1.367604	0.048031
C	-2.280623	0.104721	0.075389
C	0.055408	-0.063405	-0.087682
N	-1.183438	0.814197	0.006257
C	1.049961	0.486601	-1.115831
C	0.847862	0.028990	1.234601
O	-1.054255	2.072935	0.060758
H	-0.496060	-1.637042	-1.478819

H	-0.000269	-2.255225	0.099230
H	-2.180392	-1.818395	1.040457
H	-2.694974	-1.899657	-0.639523
H	-3.227236	0.615323	0.195745
H	0.765459	0.251650	-2.147362
H	1.057110	1.576427	-1.007265
C	2.399220	-0.126258	-0.695675
H	2.534347	-1.106336	-1.168973
H	3.244633	0.493817	-1.010193
C	2.316786	-0.284784	0.852232
H	2.599835	-1.299009	1.153818
H	3.002674	0.395878	1.366460
H	0.449838	-0.637266	2.007898
H	0.753504	1.057722	1.597423

MAMPO

C	1.482457	-1.311248	0.088562
C	2.220488	-0.644037	-1.101549
C	1.879407	0.801427	-0.941167
C	0.436487	-0.285330	0.557599
N	0.939000	1.009235	-0.062288
C	0.348266	-0.114545	2.075974
C	-0.979965	-0.615957	-0.005673
O	0.405671	2.123727	0.272883
H	2.189113	-1.511029	0.899955
H	0.991281	-2.247065	-0.180384
H	1.867860	-1.024025	-2.071478
H	3.302016	-0.821460	-1.072604
H	1.342307	0.067986	2.497970
H	-0.299577	0.726434	2.332111
H	-0.058547	-1.029656	2.517168
O	-1.304776	-1.783432	-0.203993
N	-1.789021	0.454375	-0.178763
C	-3.152184	0.332069	-0.662477
H	2.283081	1.648375	-1.481694
H	-1.376675	1.372570	-0.014066
H	-3.379779	-0.729987	-0.763172
H	-3.270966	0.818707	-1.638151
H	-3.856857	0.787235	0.042966

DiMAMPO

C	-0.837585	1.520440	-0.527694
C	-1.856265	0.911005	-1.521969
C	-2.439224	-0.210903	-0.730414
C	-0.464185	0.352472	0.416701
N	-1.718562	-0.525191	0.314031
C	-0.301530	0.682551	1.901791
C	0.692697	-0.511168	-0.175174
O	-1.923839	-1.419895	1.177599
H	-1.314849	2.315401	0.056167
H	0.024829	1.952541	-1.041166
H	-1.359318	0.545949	-2.433519
H	-2.607004	1.643970	-1.839441
H	-1.153415	1.282185	2.240468

H	-0.301954	-0.252048	2.467235
H	0.613178	1.233934	2.119082
O	0.439260	-1.576265	-0.721450
N	1.987831	-0.050986	-0.069677
C	3.057106	-0.923326	-0.545408
H	-3.327260	-0.789795	-0.945278
H	2.658634	-1.926592	-0.683562
H	3.869826	-0.941333	0.190763
H	3.463041	-0.564578	-1.501593
C	2.435634	1.278825	0.314102
H	1.605143	1.966970	0.448760
H	3.018831	1.248655	1.244916
H	3.082177	1.687892	-0.474110

DiMAPO

C	-0.631084	-1.626173	-1.164329
C	-1.423269	-2.550096	-0.204065
C	-1.050186	-2.046056	1.148359
C	-0.148121	-0.443539	-0.305194
N	-0.379302	-0.932607	1.113677
C	1.339213	-0.098849	-0.615402
O	1.705631	-0.139825	-1.783652
C	3.510298	0.615010	0.277921
H	-1.236412	-1.246469	-1.987320
H	0.231588	-2.141090	-1.588935
H	-1.166098	-3.608244	-0.331155
H	-2.509524	-2.472832	-0.353683
H	3.774390	0.498203	-0.773868
H	4.155170	-0.028535	0.887132
C	-1.017735	0.839732	-0.554609
O	-1.642530	0.971683	-1.597598
C	-1.744528	2.984203	0.379021
H	-1.222655	3.771709	0.929868
H	-1.850131	3.279566	-0.666005
H	-1.301689	-2.466533	2.114473
O	0.022764	-0.242900	2.133459
H	-2.747851	2.857585	0.806915
N	-0.967653	1.757363	0.438795
H	-0.558066	1.455546	1.320829
N	2.115772	0.242003	0.436390
H	1.680323	0.218748	1.357613
H	3.674770	1.657967	0.574214

EMAPO

C	-0.471109	1.374712	-1.327635
C	-0.355034	2.713529	-0.548491
C	-0.311145	2.278197	0.878205
C	-0.056959	0.285915	-0.319560
N	-0.163647	0.990476	1.016465
C	-1.001659	-0.928236	-0.271478
O	-0.656398	-2.075573	-0.422482
H	0.182029	1.325483	-2.199296
H	-1.503273	1.216973	-1.644448
H	-1.200330	3.381997	-0.749998

H	0.554908	3.268059	-0.818900	C	0.890142	-0.070048	0.465788
C	1.404127	-0.211096	-0.564397	N	0.831412	-0.982743	-0.750588
O	1.885063	-0.148078	-1.690050	C	2.257701	-0.268513	1.114251
C	3.356959	-1.267932	0.482510	C	0.746934	1.403307	-0.021263
H	3.318883	-2.349019	0.662623	O	1.679078	-0.831121	-1.686728
H	3.769187	-1.088942	-0.511294	H	0.033519	-0.783151	2.344101
H	-0.356184	2.892994	1.768169	H	-1.101257	0.200306	1.383100
O	-0.073698	0.304429	2.091006	H	-1.960932	-1.653705	0.432177
H	4.006463	-0.807028	1.234789	H	-0.771191	-2.723442	1.210433
O	-2.268582	-0.534443	-0.055042	H	2.350623	-1.295068	1.490294
N	2.028482	-0.685510	0.531945	H	3.044074	-0.076626	0.382009
H	1.499910	-0.678490	1.402464	H	2.377475	0.433648	1.942846
C	-3.231263	-1.598804	0.062240	O	1.641757	2.221285	0.215514
H	-2.970308	-2.250607	0.899387	N	-0.393092	1.685311	-0.673513
H	-4.187567	-1.106956	0.239709	H	-0.492901	2.661417	-0.923269
H	-3.262146	-2.187615	-0.857902	H	-1.283083	1.081321	-0.722263

Miscellaneous

Superoxide Radical Anion

O	0.000000	0.000000	0.676584
O	0.000000	0.000000	-0.676584

TS and Displacement Structures

AMPO-O₂ TS

C	-0.273063	-1.151028	-1.293222
C	1.075394	-1.781248	-0.862223
C	1.471406	-0.910373	0.298582
C	-0.858505	-0.501003	-0.006634
N	0.321740	-0.479807	0.899083
C	-1.962697	-1.330282	0.654857
C	-1.390506	0.932284	-0.304514
O	0.261316	0.100360	2.052006
H	-0.968132	-1.878505	-1.727630
H	-0.071528	-0.373001	-2.031758
H	1.821988	-1.737095	-1.662325
H	0.959185	-2.834101	-0.560773
H	-1.670475	-2.386652	0.710424
H	-2.122592	-0.958538	1.671538
H	-2.892316	-1.228294	0.091143
O	-2.605305	1.107598	-0.482832
N	-0.458863	1.890449	-0.429516
H	-0.848941	2.806193	-0.619122
H	0.592383	1.828949	-0.141381
H	2.269918	-1.160133	0.989262
O	2.191170	0.477067	-0.594140
O	2.092594	1.627049	0.159038

AMPO-O₂ neg displacement

C	-0.304935	-0.550903	1.328443
C	-0.892199	-1.802894	0.616599
C	-0.116830	-1.874989	-0.652357

AMPO-O₂ pos displacement

C	-0.379056	-1.129754	-1.279824
C	1.057672	-1.650943	-1.019375
C	1.590293	-0.670113	0.026237
C	-0.852609	-0.468983	0.054572
N	0.402759	-0.445351	0.840008
C	-1.903795	-1.297674	0.795699
C	-1.418453	0.969835	-0.242040
O	0.453109	-0.301069	2.108864
H	-1.057110	-1.933197	-1.587521
H	-0.361974	-0.382869	-2.076444
H	1.676296	-1.663134	-1.922996
H	1.047524	-2.662043	-0.592835
H	-1.626878	-2.360448	0.831145
H	-1.998654	-0.933078	1.822682
H	-2.858121	-1.173150	0.279975
O	-2.596030	1.007500	-0.676102
N	-0.562932	1.960974	-0.045805
H	-1.026366	2.827339	-0.331156
H	1.036400	1.849862	0.151671
H	2.382360	-1.025188	0.696691
O	2.005855	0.468835	-0.712861
O	2.054994	1.616274	0.174817

DEPMPO-O₂ TS

C	-1.107591	-1.813939	0.086558
C	-2.626895	-1.648225	0.304516
C	-2.805755	-0.142910	0.313293
C	-0.518397	-0.557357	0.773308
N	-1.614641	0.396695	0.691281
O	-1.471544	1.635368	1.225435
H	-0.889822	-1.798662	-0.985692
H	-0.700740	-2.739183	0.508642
H	-2.933708	-2.060517	1.276723

H	-3.237521	-2.124464	-0.468827
O	-3.206406	0.283377	-1.241354
O	-4.351548	-0.289852	-1.579297
H	-3.684180	0.266536	0.819135
C	-0.113232	-0.758797	2.246935
H	0.846642	-1.272721	2.356523
H	-0.068832	0.232965	2.705159
H	-0.889192	-1.343209	2.758520
P	0.945781	0.062128	-0.214353
O	0.714200	0.325834	-1.663916
O	2.017492	-1.155278	0.073083
O	1.716795	1.250132	0.585443
C	3.248384	-1.156868	-0.661056
H	3.873303	-0.320783	-0.320725
H	3.037719	-1.010817	-1.727167
C	1.236471	2.624644	0.493655
H	1.587473	3.093138	1.420262
H	0.136387	2.601473	0.513805
C	1.817690	3.326284	-0.724844
H	1.464009	2.848202	-1.642471
H	1.500051	4.377689	-0.731249
H	2.915339	3.299602	-0.716642
C	3.944044	-2.486924	-0.418049
H	4.898588	-2.523886	-0.957685
H	4.142831	-2.629960	0.649737
H	3.317203	-3.316291	-0.762756

DEPMPO-O₂ neg displacement

C	-1.164461	-1.744057	-0.029055
C	-2.664592	-1.585766	0.280496
C	-2.897582	-0.075104	0.241137
C	-0.545559	-0.514501	0.674931
N	-1.603394	0.489846	0.526097
O	-1.492067	1.654134	1.146137
H	-1.000636	-1.681154	-1.108999
H	-0.729597	-2.680651	0.335120
H	-2.904869	-1.985292	1.274395
H	-3.333006	-2.042781	-0.456992
O	-3.289509	0.356477	-1.069784
O	-4.449963	-0.346140	-1.423021
H	-3.658096	0.270637	0.961165
C	-0.214540	-0.748089	2.162716
H	0.686275	-1.355209	2.293312
H	-0.078710	0.225348	2.640564
H	-1.056530	-1.255345	2.648640
P	0.976622	0.051234	-0.239443
O	0.832087	0.349996	-1.691881
O	1.989600	-1.197537	0.092142
O	1.729518	1.211045	0.622899
C	3.256575	-1.236828	-0.580630
H	3.880322	-0.407710	-0.222237
H	3.100258	-1.104197	-1.657420
C	1.337748	2.604903	0.481861
H	1.641635	3.067438	1.427531
H	0.245949	2.659488	0.418409

C	2.041943	3.261965	-0.696157
H	1.732680	2.791452	-1.633117
H	1.783307	4.328430	-0.733721
H	3.131842	3.175561	-0.602159
C	3.909357	-2.576317	-0.280569
H	4.887351	-2.642956	-0.772906
H	4.053849	-2.703246	0.797820
H	3.281748	-3.398286	-0.640764

DEPMPO-O₂ pos displacement

C	-1.368479	-1.457250	0.465368
C	-2.828149	-1.000397	0.723768
C	-2.705553	0.478170	0.637201
C	-0.512907	-0.251282	0.915209
N	-1.458994	0.887247	0.759112
O	-0.995136	2.108922	0.850895
H	-1.247169	-1.623220	-0.609410
H	-1.086280	-2.373821	0.993018
H	-3.181179	-1.322573	1.719006
H	-3.541295	-1.369684	-0.041013
O	-3.966328	0.315238	-1.555107
O	-4.541677	-0.868801	-1.586881
H	-3.497749	1.208620	0.659341
C	-0.065010	-0.299126	2.385578
H	0.739764	-1.024402	2.536278
H	0.276268	0.694924	2.684644
H	-0.918465	-0.582424	3.013318
P	0.947409	0.004450	-0.202402
O	0.682440	0.202716	-1.652568
O	1.754505	-1.375115	0.163105
O	1.971917	1.076773	0.464131
C	2.922911	-1.704819	-0.603130
H	3.739182	-1.027087	-0.321155
H	2.711061	-1.560038	-1.668678
C	1.896887	2.481751	0.097165
H	2.241572	3.017367	0.988321
H	0.850290	2.744279	-0.074251
C	2.787971	2.776260	-1.099950
H	2.419554	2.247135	-1.983224
H	2.783911	3.853810	-1.310549
H	3.823349	2.467920	-0.908243
C	3.288826	-3.150135	-0.308083
H	4.187972	-3.437123	-0.866895
H	3.485081	-3.289217	0.760637
H	2.471189	-3.818865	-0.596256

DMPO-O₂ TS

C	-0.488861	-1.518504	-0.626268
C	0.854865	-0.989510	-1.195581
C	0.804166	0.494041	-0.954828
C	-1.071664	-0.351586	0.205946
N	-0.413861	0.821512	-0.440792
C	-0.657279	-0.408516	1.687997
C	-2.587514	-0.190618	0.069721

O	-0.869005	2.032913	-0.224194
O	2.080513	0.754905	0.303285
H	-0.352759	-2.422008	-0.019437
H	-1.183050	-1.770960	-1.439024
H	0.985073	-1.243089	-2.255645
H	1.712312	-1.369583	-0.613664
H	1.203209	1.221611	-1.655545
H	0.423709	-0.566858	1.781840
H	-0.907988	0.549938	2.156624
H	-1.192340	-1.212198	2.215562
H	-3.114377	-1.004075	0.585261
H	-2.881255	0.771032	0.499634
H	-2.889117	-0.194120	-0.985403
O	2.534908	-0.378083	0.882587

DMPO-O₂ neg displacement

C	-0.138558	-1.436155	0.073985
C	0.851723	-0.844797	-0.961806
C	0.524482	0.604530	-0.910384
C	-1.265186	-0.391445	0.225301
N	-0.623602	0.858771	-0.327279
C	-1.671456	-0.115470	1.673304
C	-2.499752	-0.680261	-0.641879
O	-1.247364	1.990250	-0.198818
O	2.803461	0.734019	0.518585
H	0.391307	-1.548441	1.026042
H	-0.529857	-2.420538	-0.211465
H	0.686633	-1.261870	-1.971320
H	1.907382	-1.019030	-0.664830
H	1.067572	1.413531	-1.374852
H	-0.784249	0.083360	2.283829
H	-2.315260	0.768153	1.707247
H	-2.203472	-0.976682	2.097706
H	-3.098245	-1.496681	-0.218065
H	-3.111788	0.225673	-0.698310
H	-2.204157	-0.962099	-1.659838
O	3.412882	-0.428666	0.333193

DMPO-O₂ pos displacement

C	-0.252188	-1.543179	0.179495
C	0.890859	-1.219632	-0.808171
C	1.047138	0.294304	-0.666846
C	-1.160925	-0.283903	0.208255
N	-0.341160	0.714758	-0.529313
C	-1.429488	0.229419	1.632521
C	-2.481134	-0.471705	-0.556361
O	-0.728757	1.945726	-0.611712
O	1.739307	0.621017	0.518197
H	0.172688	-1.713519	1.173592
H	-0.817854	-2.441859	-0.099409
H	0.635477	-1.503931	-1.838016
H	1.855453	-1.644394	-0.511234
H	1.507770	0.783834	-1.540794
H	-0.473056	0.385928	2.139607

H	-1.958326	1.187555	1.587701
H	-2.034924	-0.486562	2.205370
H	-3.173109	-1.120078	-0.002845
H	-2.951789	0.506009	-0.706713
H	-2.300694	-0.919095	-1.541440
O	3.019563	-0.075370	0.456768

EMPO-O₂ TS

C	-0.719605	-0.007497	-1.490385
C	-1.209301	-1.326354	-0.846389
C	-1.503242	-0.903626	0.567178
C	-0.200102	0.856249	-0.306205
N	-0.682113	0.126102	0.874009
C	-0.727479	2.293975	-0.294756
O	-0.402060	0.611675	2.077184
H	-1.565047	0.507274	-1.957159
H	0.041937	-0.168761	-2.262563
H	-0.430664	-2.100666	-0.867843
H	-2.120530	-1.707682	-1.319993
H	-1.817756	2.255475	-0.376659
H	-0.463235	2.747130	0.663985
H	-0.307076	2.892314	-1.110398
C	1.338142	0.879938	-0.249251
O	1.851254	-0.371635	-0.116140
C	3.276897	-0.449781	-0.005914
C	3.636910	-1.911052	0.202410
O	2.048841	1.859030	-0.354185
H	3.738799	-0.042464	-0.914081
H	3.607009	0.172494	0.833187
H	4.723711	-2.024870	0.298064
H	3.163890	-2.296488	1.111167
H	3.297779	-2.520139	-0.642583
O	-3.163457	-0.297892	0.468831
O	-3.936740	-0.994344	-0.374346
H	-1.630048	-1.642116	1.355940

EMPO-O₂ neg displacement

C	-0.678475	-0.028785	-1.495677
C	-1.228010	-1.328716	-0.870427
C	-1.727229	-0.865549	0.495467
C	-0.187751	0.841437	-0.297263
N	-0.700882	0.094605	0.874067
C	-0.731943	2.274036	-0.309275
O	-0.584652	0.596876	2.060634
H	-1.487453	0.506156	-2.001659
H	0.115590	-0.209784	-2.229605
H	-0.448046	-2.093469	-0.777342
H	-2.107936	-1.714959	-1.395024
H	-1.822091	2.214493	-0.360117
H	-0.445504	2.783494	0.614390
H	-0.342476	2.840243	-1.162143
C	1.344656	0.872509	-0.230233
O	1.869380	-0.368245	-0.061785
C	3.299623	-0.434311	0.017903

C	3.675283	-1.890253	0.233255
O	2.043832	1.859623	-0.342726
H	3.735759	-0.033038	-0.905002
H	3.644109	0.200649	0.841775
H	4.764794	-1.993600	0.304809
H	3.227214	-2.271283	1.156439
H	3.321622	-2.510091	-0.597453
O	-2.957613	-0.179469	0.376030
O	-3.877572	-1.078407	-0.297062
H	-1.793343	-1.666271	1.249239

EMPO-O₂ pos displacement

C	-0.546069	-0.109585	-1.538280
C	-1.650387	-1.101979	-1.086516
C	-1.345081	-1.292732	0.355462
C	-0.143545	0.603822	-0.226654
N	-0.471963	-0.426536	0.813561
C	-0.972582	1.857158	0.064980
O	0.005354	-0.265250	2.007478
H	-0.901624	0.605590	-2.287779
H	0.315783	-0.643993	-1.951869
H	-1.619134	-2.040535	-1.658004
H	-2.667914	-0.650701	-1.189715
H	-2.034156	1.618339	-0.054848
H	-0.789157	2.174258	1.094898
H	-0.691735	2.671360	-0.611338
C	1.352836	0.901238	-0.116995
O	2.097624	-0.224325	-0.240333
C	3.507392	-0.060997	-0.037331
C	4.137274	-1.441669	-0.098853
O	1.848889	1.999198	0.024289
H	3.912983	0.607356	-0.806745
H	3.672709	0.418139	0.933450
H	5.220239	-1.371039	0.059034
H	3.712564	-2.090111	0.673794
H	3.959508	-1.909436	-1.073390
O	-3.884095	-0.422743	0.708372
O	-4.201549	0.100110	-0.467855
H	-1.755136	-2.030916	1.027107

CPCOMPO-O₂ TS

C	0.200320	-0.569863	-1.413009
C	1.495592	-1.207645	-0.868486
C	1.653597	-0.537319	0.477984
C	-0.608325	-0.272217	-0.132736
N	0.420869	-0.150397	0.890128
C	-1.670509	-1.301719	0.310511
C	-1.444692	1.018637	-0.280843
O	0.040798	0.077305	2.156247
H	-0.343832	-1.212408	-2.116740
H	0.435789	0.374618	-1.913316
H	2.369715	-1.039692	-1.505612
H	1.374360	-2.293510	-0.735219
H	-1.506958	-2.303102	-0.101114

H	-1.584225	-1.315320	1.404615
O	-1.062580	2.142348	-0.477921
C	-3.002151	-0.692505	-0.124165
H	-3.334351	-1.054001	-1.108214
H	-3.818063	-0.848429	0.590428
H	2.276471	-1.015834	1.235758
O	2.670851	0.805917	0.172326
O	3.815597	0.388004	-0.353712
O	-2.784414	0.728456	-0.221567

CPCOMPO-O₂ neg displacement

C	0.269668	-0.429651	-1.300802
C	1.516238	-1.105636	-0.675793
C	1.386702	-0.731194	0.756186
C	-0.713190	-0.265561	-0.122952
N	0.178626	-0.308510	1.070248
C	-1.832983	-1.303598	0.045408
C	-1.487891	1.060104	-0.186950
O	-0.336449	-0.035778	2.229740
H	-0.169271	-0.992038	-2.133429
H	0.552979	0.563517	-1.662625
H	2.474800	-0.726272	-1.092360
H	1.487177	-2.201328	-0.811047
H	-1.617460	-2.259491	-0.441656
H	-1.955381	-1.452675	1.123198
O	-1.061113	2.182059	-0.153111
C	-3.062571	-0.600909	-0.535127
H	-3.196512	-0.806165	-1.606274
H	-3.995833	-0.843062	-0.017205
H	2.107461	-0.888381	1.541683
O	3.532478	0.730724	0.332507
O	4.016777	0.318371	-0.823445
O	-2.825965	0.807641	-0.369671

CPCOMPO-O₂ pos displacement

C	0.203091	-0.742241	-1.267955
C	1.478278	-1.297372	-0.611479
C	1.785403	-0.287486	0.497805
C	-0.589162	-0.213867	-0.054282
N	0.473615	0.247936	0.840078
C	-1.526155	-1.230193	0.631395
C	-1.563003	0.917100	-0.441015
O	0.164034	0.620203	2.051111
H	-0.363599	-1.482908	-1.845602
H	0.453359	0.097082	-1.923690
H	2.362141	-1.313177	-1.259890
H	1.300366	-2.299315	-0.197094
H	-1.224414	-2.270483	0.476813
H	-1.497612	-0.995496	1.701252
O	-1.314923	2.028063	-0.827157
C	-2.898864	-0.915999	0.038689
H	-3.116648	-1.514739	-0.856707
H	-3.728262	-1.036874	0.743602
H	2.264035	-0.742523	1.381993

O	2.587514	0.768022	0.008467
O	3.784911	0.167263	-0.494136
O	-2.859312	0.471853	-0.345807

TAMPO-O₂ TS

C	0.209580	-0.390950	-1.468441
C	1.503865	-1.090514	-1.004516
C	1.658480	-0.590364	0.413949
C	-0.604194	-0.245374	-0.166529
N	0.426385	-0.252811	0.867230
C	-1.657851	-1.338546	0.153302
C	-1.445028	1.057425	-0.177578
O	0.052469	-0.183001	2.152626
H	-0.333572	-0.943094	-2.246426
H	0.445362	0.607700	-1.849443
H	2.380836	-0.845624	-1.612545
H	1.384249	-2.185091	-1.006181
H	-1.482527	-2.278353	-0.380606
H	-1.553908	-1.489474	1.235137
O	-1.047434	2.203399	-0.304332
C	-3.035206	-0.728140	-0.165315
H	-3.396679	-1.018320	-1.166851
H	-3.805883	-1.024737	0.559850
N	-2.768531	0.698108	-0.091369
H	2.279590	-1.157588	1.109499
O	2.685975	0.779899	0.275785
O	3.831372	0.421055	-0.294730
H	-3.479374	1.405450	-0.217476

TAMPO-O₂ neg displacement

C	0.246007	-0.203575	-1.346364
C	1.522832	-0.911792	-0.824719
C	1.377648	-0.778201	0.647554
C	-0.734882	-0.228317	-0.156929
N	0.166507	-0.421867	1.019221
C	-1.822006	-1.323193	-0.132785
C	-1.541843	1.081674	-0.046839
O	-0.343422	-0.325021	2.205846
H	-0.181128	-0.667539	-2.243719
H	0.486054	0.839081	-1.577343
H	2.472637	-0.441286	-1.167800
H	1.545434	-1.972940	-1.129964
H	-1.572503	-2.190136	-0.752025
H	-1.920148	-1.631924	0.912724
O	-1.111838	2.213234	0.078094
C	-3.119218	-0.624028	-0.585169
H	-3.280437	-0.722713	-1.671446
H	-4.007483	-1.024303	-0.080023
N	-2.870127	0.754906	-0.202768
H	2.123091	-0.996197	1.394453
O	3.745511	0.584629	0.462001
O	4.113285	0.389963	-0.793985
H	-3.539701	1.498839	-0.344173

TAMPO-O₂ pos displacement

C	0.213387	-0.551259	-1.358768
C	1.488634	-1.194563	-0.788835
C	1.795744	-0.352974	0.453767
C	-0.586430	-0.200427	-0.087898
N	0.476591	0.115464	0.871800
C	-1.519119	-1.317261	0.446222
C	-1.557803	0.981264	-0.325775
O	0.170901	0.322907	2.118908
H	-0.352239	-1.201109	-2.038429
H	0.463100	0.374795	-1.885322
H	2.375108	-1.114699	-1.429179
H	1.312021	-2.246191	-0.522793
H	-1.211387	-2.319072	0.131748
H	-1.473181	-1.249572	1.538316
O	-1.283474	2.128524	-0.629175
C	-2.931197	-0.951667	-0.046097
H	-3.172463	-1.446319	-1.001722
H	-3.713577	-1.225126	0.674325
N	-2.838417	0.490889	-0.199139
H	2.274445	-0.931056	1.263584
O	2.590885	0.761998	0.123385
O	3.799735	0.232616	-0.449904
H	-3.612716	1.066846	-0.500572

TFMPO-O₂ TS

C	0.266274	-1.292814	0.725074
C	1.272456	-1.385211	-0.443435
C	1.510558	0.068004	-0.761986
C	-0.468468	0.051528	0.503215
N	0.403769	0.762093	-0.448925
C	-0.670791	0.906056	1.760080
C	-1.836757	-0.196951	-0.157232
O	0.148039	2.039471	-0.747794
H	0.810357	-1.239017	1.672888
H	-0.417828	-2.146212	0.780686
H	0.838198	-1.909842	-1.306249
H	2.205446	-1.884650	-0.167805
H	0.273601	0.946056	2.311395
H	-0.916502	1.917672	1.425667
H	-1.457847	0.510047	2.411954
H	2.025302	0.367395	-1.671895
O	2.876639	0.472533	0.338095
O	3.911233	-0.320267	0.120152
F	-1.727269	-0.870466	-1.328590
F	-2.542489	0.920163	-0.403861
F	-2.631802	-0.975661	0.648885

TFMPO-O₂ neg displacement

C	0.470828	-1.257957	0.248617
C	1.339005	-0.962853	-0.998671
C	1.203729	0.508460	-1.126040
C	-0.434086	-0.017823	0.441183

N	0.191504	1.011350	-0.454701	H	0.051668	3.375074	0.933261
C	-0.464176	0.533492	1.866372	H	-1.409793	2.388965	1.270287
C	-1.857005	-0.295111	-0.053081	H	3.641776	-1.418985	-1.119357
O	-0.242281	2.233219	-0.415751	H	4.165798	-1.421807	0.570191
H	1.139270	-1.341820	1.108768	H	5.175881	0.878603	0.256715
H	-0.108418	-2.182987	0.172148	H	4.642999	0.870555	-1.435900
H	0.971396	-1.490390	-1.894535	H	5.883349	-0.282762	-0.888656
H	2.389089	-1.244190	-0.792503	C	-0.847003	-0.803333	0.880371
H	0.568452	0.671274	2.199274	O	-1.166599	-1.012004	2.035275
H	-0.966968	1.502988	1.869567	O	-1.504143	-1.261806	-0.184123
H	-0.974839	-0.159941	2.543375	C	-2.834583	-1.763985	0.041522
H	1.750056	1.161894	-1.790785	H	-2.769874	-2.797899	0.406368
O	3.304146	0.498192	0.423836	H	-3.309557	-1.144080	0.804259
O	3.846557	-0.708613	0.379052	C	-3.565365	-1.654814	-1.284512
F	-1.877327	-0.685951	-1.349390	H	-3.074454	-2.257228	-2.056982
F	-2.693931	0.752167	0.061880	H	-4.601518	-2.000784	-1.175137
F	-2.420488	-1.313762	0.665312	H	-3.562813	-0.607560	-1.598301

TFMPO-O₂ pos displacement

C	0.314567	-1.327078	0.608602	C	-0.454804	1.368046	-1.422875
C	1.319302	-1.383974	-0.559480	C	0.107018	2.652180	-0.741079
C	1.683054	0.086234	-0.744709	C	0.603469	2.184029	0.638310
C	-0.419284	0.032433	0.455281	C	-0.248960	0.247833	-0.372428
N	0.396643	0.742992	-0.560187	N	-0.277969	1.031096	0.884665
C	-0.513793	0.850406	1.749959	C	-1.352040	-0.802668	-0.344232
C	-1.822640	-0.186801	-0.122075	O	-1.248690	-1.992581	-0.520660
O	0.243476	2.019329	-0.742356	O	-2.560423	-0.212196	-0.086221
H	0.864239	-1.318858	1.553556	C	-3.663240	-1.113964	0.055258
H	-0.380870	-2.172857	0.628977	C	-4.882728	-0.285538	0.423724
H	0.866824	-1.804982	-1.464901	H	0.097901	1.093168	-2.322271
H	2.245421	-1.902478	-0.296778	H	-1.516250	1.482792	-1.662507
H	0.501960	0.977653	2.131931	H	-0.678627	3.406685	-0.610519
H	-0.931318	1.836560	1.532537	H	0.930850	3.092284	-1.305467
H	-1.133205	0.343544	2.498408	H	-3.427586	-1.853909	0.828112
H	2.099471	0.333558	-1.733583	H	-3.813173	-1.662170	-0.882959
O	2.542813	0.528215	0.291101	H	-5.104609	0.450151	-0.357226
O	3.684783	-0.355385	0.311114	H	-4.711363	0.253833	1.360972
F	-1.805076	-0.903115	-1.271367	H	-5.759318	-0.932982	0.548498
F	-2.479778	0.961975	-0.383150	C	1.190294	-0.384489	-0.621343
F	-2.609017	-0.887491	0.750830	O	1.412817	-0.871901	-1.753082

DEPO-O₂ TS

C	0.476684	1.274154	1.475703	O	1.488263	-1.123623	0.558729
C	-0.400927	2.381000	0.831861	C	2.507359	-2.093873	0.398391
C	-0.537115	1.957810	-0.610490	H	2.309979	-2.861972	1.158948
C	0.349970	0.098549	0.480680	H	2.418344	-2.548653	-0.594772
N	0.155212	0.804846	-0.796417	C	3.906582	-1.505041	0.589320
C	1.595760	-0.779682	0.325612	H	3.991376	-1.026642	1.572073
O	1.621366	-1.986997	0.425510	H	4.674084	-2.289919	0.512688
O	2.698754	-0.034638	0.086262	H	4.091788	-0.742903	-0.171586
C	3.875682	-0.774168	-0.265888	H	0.494541	2.896558	1.461615
C	4.959552	0.234840	-0.603091	O	1.948069	1.779812	0.646899
H	0.140602	0.984623	2.473466	O	2.132631	0.941663	-0.561463
H	1.523955	1.584533	1.525475				

O -0.463898 0.532191 2.047482
DEPO-O₂ pos displacement

C -0.452823 1.204388 -1.410468
C 0.516786 2.226306 -0.762238
C 0.376627 1.914434 0.685667
C -0.445177 0.044227 -0.391111
N -0.217985 0.764272 0.904521
C -1.742442 -0.753546 -0.251250
O -1.833848 -1.959807 -0.272814
O -2.804939 0.069073 -0.098058
C -4.049478 -0.582789 0.201601
C -5.089811 0.502577 0.414323
H -0.135286 0.858686 -2.396185
H -1.466048 1.611535 -1.479619
H 0.242768 3.262917 -1.000662
H 1.572212 2.047341 -1.080593
H -3.915453 -1.200793 1.095355
H -4.317238 -1.250087 -0.625724
H -5.203883 1.116131 -0.485932
H -4.798030 1.157668 1.241196
H -6.061008 0.052223 0.651519
C 0.717661 -0.917262 -0.734453
O 0.858220 -1.366437 -1.854937
O 1.534944 -1.123174 0.288503
C 2.826702 -1.700401 -0.020213
H 2.681220 -2.750041 -0.304121
H 3.242842 -1.145579 -0.864003
C 3.689534 -1.525476 1.214597
H 3.244098 -2.023171 2.083923
H 4.681786 -1.959509 1.034478
H 3.791772 -0.452192 1.410645
H 0.702212 2.503552 1.529116
O 3.119938 1.584185 0.563637
O 3.311931 1.405892 -0.737998
O -0.538940 0.183601 2.009195

CPPO-O₂ TS

C -0.172339 -1.447623 0.183996
C -1.428499 -1.279407 -0.699887
C -1.600157 0.219929 -0.716068
C 0.643847 -0.155696 -0.045969
N -0.366993 0.764982 -0.597220
C 1.821520 -0.313337 -1.043878
O -0.045393 2.039993 -0.802179
H 0.402249 -2.354700 -0.048612
H -0.484565 -1.507677 1.231848
H -2.319267 -1.758363 -0.279913
H -1.266751 -1.666085 -1.717702
H 1.617475 -1.058432 -1.823656
H 1.943421 0.668042 -1.519885
C 3.034386 -0.645370 -0.169431
H 2.986192 -1.694451 0.159926
H 3.997647 -0.513054 -0.680977
H -2.257664 0.687212 -1.448370

O -2.544586 0.534043 0.717627
O -3.611608 -0.273777 0.782571
C 1.325311 0.450805 1.219078
H 1.033152 1.505405 1.240617
H 0.965742 -0.033963 2.133696
C 2.858259 0.299014 1.039831
H 3.306230 1.273024 0.803096
H 3.363822 -0.073789 1.940285

CPPO-O₂ neg displacement

C -0.355058 -1.357182 0.028340
C -1.481082 -0.883248 -0.922012
C -1.266045 0.588678 -0.923220
C 0.716374 -0.251346 -0.016369
N -0.078955 0.934164 -0.481573
C 1.889795 -0.477116 -1.016565
O 0.472528 2.110155 -0.429967
H 0.056882 -2.341649 -0.227424
H -0.774298 -1.416737 1.039030
H -2.487133 -1.133015 -0.527230
H -1.369659 -1.311454 -1.934308
H 1.683355 -1.287098 -1.726108
H 2.019095 0.455201 -1.577710
C 3.135712 -0.713992 -0.148327
H 3.167158 -1.754452 0.208734
H 4.075193 -0.524417 -0.683922
H -1.918206 1.346924 -1.328746
O -3.348916 0.582110 0.741220
O -3.922114 -0.606573 0.619869
C 1.403023 0.063157 1.341217
H 0.957367 0.954600 1.788875
H 1.252368 -0.782670 2.025097
C 2.900016 0.240803 1.034119
H 3.073140 1.272582 0.706517
H 3.549031 0.038979 1.896141

CPPO-O₂ pos displacement

C -0.151765 -1.451826 -0.032988
C -1.465579 -1.224327 -0.810646
C -1.747463 0.255945 -0.556603
C 0.621282 -0.109687 -0.120970
N -0.410730 0.819126 -0.633954
C 1.837599 -0.149750 -1.077250
O -0.176216 2.091563 -0.699551
H 0.439446 -2.290464 -0.425159
H -0.396190 -1.673189 1.010114
H -2.314229 -1.773878 -0.391681
H -1.350764 -1.431948 -1.883004
H 1.660991 -0.785716 -1.953435
H 2.009696 0.876473 -1.427269
C 2.997325 -0.621061 -0.193301
H 2.915793 -1.703847 -0.021186
H 3.986954 -0.439707 -0.633048
H -2.403779 0.725918 -1.307035

O	-2.242433	0.459411	0.751603
O	-3.409219	-0.388228	0.904912
C	1.244185	0.391924	1.217728
H	1.024179	1.460730	1.291215
H	0.779484	-0.104774	2.074288
C	2.775192	0.144158	1.132617
H	3.314575	1.100086	1.100493
H	3.167244	-0.407796	1.996146

MAMPO-O₂ TS

C	0.670096	-0.656098	-1.561253
C	2.071789	-0.238799	-1.031961
C	1.898772	-0.215937	0.452505
C	-0.170075	-1.069262	-0.321971
N	0.774065	-0.824362	0.821573
C	-0.551343	-2.549413	-0.301958
C	-1.454831	-0.205992	-0.135186
O	0.415273	-1.146004	2.017451
H	0.730650	-1.488067	-2.271930
H	0.205939	0.187803	-2.075750
H	2.326841	0.765352	-1.389930
H	2.854778	-0.948627	-1.337664
H	0.336841	-3.163891	-0.495955
H	-0.954090	-2.802153	0.680260
H	-1.311585	-2.757194	-1.059497
O	-2.566872	-0.739281	-0.043239
N	-1.277819	1.130201	-0.116672
C	-2.422038	1.990092	0.088296
H	2.699093	-0.190812	1.178630
O	1.629827	1.756800	0.728329
O	1.132608	2.334576	-0.390849
H	-0.340335	1.608692	-0.217167
H	-2.909056	1.793266	1.052810
H	-3.182891	1.852234	-0.692771
H	-2.070810	3.026234	0.070285

MAMPO-O₂ neg displacement

C	-0.606846	-0.939812	-1.582139
C	0.695752	-1.652644	-1.135020
C	0.484393	-1.842110	0.329121
C	-1.226155	-0.357370	-0.288105
N	-0.529850	-1.160430	0.794227
C	-2.728788	-0.574409	-0.156542
C	-0.899447	1.154495	-0.095778
O	-0.954912	-1.074876	1.997906
H	-1.309350	-1.658443	-2.021751
H	-0.418902	-0.162249	-2.328522
H	1.583173	-1.023112	-1.288553
H	0.850113	-2.602230	-1.666078
H	-2.969937	-1.629490	-0.333595
H	-3.047487	-0.301145	0.850599
H	-3.261780	0.050448	-0.876757
O	-1.815807	1.985271	-0.065807
N	0.400030	1.489956	-0.015191

C	0.766220	2.881638	0.151172
H	1.131108	-2.364082	1.016930
O	3.107162	-0.668152	0.531198
O	2.865562	0.358134	-0.291640
H	1.220989	0.835492	-0.104351
H	0.316144	3.304986	1.057985
H	0.432703	3.496906	-0.696324
H	1.855165	2.924474	0.227664

MAMPO-O₂ pos displacement

C	-0.647485	0.653609	-1.526464
C	-2.079888	0.278705	-1.079720
C	-1.956267	-0.213421	0.371981
C	0.135865	1.030763	-0.234309
N	-0.776784	0.563498	0.837724
C	0.357133	2.537780	-0.078557
C	1.508949	0.287240	-0.132529
O	-0.525350	0.760210	2.074795
H	-0.635980	1.488665	-2.238339
H	-0.193575	-0.219269	-1.994724
H	-2.502687	-0.511065	-1.703164
H	-2.738783	1.158006	-1.106617
H	-0.581627	3.079134	-0.251870
H	0.707214	2.751695	0.934555
H	1.116404	2.880500	-0.785515
O	2.575088	0.921300	-0.156064
N	1.406421	-1.044897	-0.035858
C	2.610312	-1.834726	0.070123
H	-2.793339	0.087392	1.017013
O	-1.843588	-1.582757	0.541690
O	-0.901082	-2.108338	-0.461708
H	0.407436	-1.547011	-0.118797
H	3.194560	-1.573000	0.964351
H	3.276335	-1.698156	-0.795641
H	2.324334	-2.890122	0.132838

DiMAMPO-O₂ TS

C	0.223323	-1.976689	-0.973494
C	1.453969	-1.155776	-1.417419
C	1.843058	-0.358955	-0.177896
C	-0.339690	-1.179614	0.228364
N	0.908088	-0.619720	0.774291
C	-1.002791	-2.057505	1.299332
C	-1.456825	-0.211451	-0.316636
O	0.995932	-0.232522	2.060475
H	0.535860	-2.964531	-0.613419
H	-0.519446	-2.113826	-1.761090
H	1.205005	-0.463637	-2.231839
H	2.277796	-1.787526	-1.772514
H	-0.335279	-2.885013	1.565270
H	-1.161266	-1.460607	2.201012
H	-1.951671	-2.458133	0.929196
O	-2.269577	-0.705491	-1.113853
N	-1.569251	1.096754	0.070533

C	-0.724427	1.842022	1.002914
H	2.870772	-0.326790	0.191093
O	1.849184	1.240281	-0.754443
O	2.859858	1.930061	-0.248939
H	-0.090034	1.173834	1.610583
H	-1.386402	2.421378	1.664858
H	-0.077858	2.536471	0.453289
C	-2.601594	1.898475	-0.565497
H	-3.157293	1.273188	-1.263296
H	-3.287375	2.309273	0.190500
H	-2.147977	2.745011	-1.101335

DiMAMPO-O₂ neg displacement

C	-0.404104	-1.530281	-1.400497
C	1.045145	-0.999377	-1.455402
C	1.423979	-0.890481	-0.009330
C	-0.911909	-1.067559	-0.013951
N	0.374376	-1.026756	0.763672
C	-1.879816	-2.033331	0.667161
C	-1.630908	0.306479	-0.214654
O	0.319292	-1.033675	2.061063
H	-0.407810	-2.627440	-1.423387
H	-1.048678	-1.173513	-2.206849
H	1.125629	-0.016783	-1.933762
H	1.720806	-1.667807	-2.003691
H	-1.460502	-3.045623	0.664476
H	-2.022054	-1.730277	1.707460
H	-2.835182	-2.028425	0.138461
O	-2.697161	0.250607	-0.844673
N	-1.097905	1.501845	0.171109
C	0.063873	1.749374	1.046686
H	2.441419	-0.776826	0.376403
O	3.008890	1.149216	-0.501317
O	3.960124	0.354620	-0.017879
H	0.124466	0.983329	1.822747
H	-0.096621	2.723456	1.522463
H	1.008653	1.759598	0.486634
C	-1.771808	2.707492	-0.293843
H	-2.501860	2.438991	-1.055742
H	-2.289412	3.214011	0.534418
H	-1.030035	3.401652	-0.707664

DiMAMPO-O₂ pos displacement

C	1.171377	-1.775578	-0.743077
C	1.897738	-0.579177	-1.409554
C	1.771464	0.607904	-0.428328
C	0.273481	-1.136235	0.343681
N	1.177970	-0.038706	0.753875
C	-0.009622	-2.058583	1.533089
C	-1.106783	-0.765576	-0.321316
O	1.225390	0.450034	1.946448
H	1.893593	-2.430642	-0.239931
H	0.586706	-2.368442	-1.446953
H	1.412334	-0.289646	-2.346631

H	2.946422	-0.811474	-1.628578
H	0.931755	-2.421866	1.959561
H	-0.549348	-1.525803	2.320730
H	-0.609990	-2.912988	1.202371
O	-1.517523	-1.514768	-1.219632
N	-1.860141	0.274440	0.134586
C	-1.429524	1.305320	1.091601
H	2.701143	1.094759	-0.103838
O	0.924704	1.545399	-1.017881
O	0.918945	2.756811	-0.229554
H	-0.856665	0.863010	1.906660
H	-2.340908	1.758948	1.503194
H	-0.779883	2.063768	0.614462
C	-3.052108	0.618549	-0.624221
H	-3.278764	-0.193074	-1.314266
H	-3.898694	0.776724	0.058323
H	-2.890756	1.547045	-1.190624

DiMAPO-O₂ TS

C	0.105246	-0.789556	-1.571272
C	0.667636	-2.166449	-1.146572
C	1.090699	-1.905930	0.262028
C	-0.361280	-0.111146	-0.251650
N	0.428708	-0.874099	0.777537
C	0.026516	1.411773	-0.219330
O	0.434427	-0.502339	1.995965
H	-0.708531	-0.869837	-2.297906
H	0.910509	-0.185460	-1.991603
H	1.511301	-2.476749	-1.772352
H	-0.107671	-2.942246	-1.180709
O	-0.882992	2.293322	-0.309943
N	1.320866	1.637008	-0.181441
H	2.477245	0.640574	0.318386
H	1.519008	-2.616207	0.954173
O	2.957822	-1.106182	-0.192587
O	3.172045	-0.056746	0.658447
C	1.689032	3.041170	-0.213843
H	2.782356	3.125045	-0.163543
H	1.345876	3.545056	-1.132244
H	1.258582	3.610346	0.625774
C	-1.846829	-0.506080	0.010833
O	-2.150637	-1.700460	0.095759
N	-2.724992	0.513193	0.077652
H	-2.287473	1.449644	-0.029567
C	-4.136834	0.301362	0.287014
H	-4.479870	0.786428	1.211507
H	-4.730727	0.703072	-0.546670
H	-4.313111	-0.774006	0.364154

DiMAPO-O₂ neg displacement

C	0.393207	-1.070451	-1.134062
C	0.869928	-2.311397	-0.330420
C	0.565289	-1.949138	1.079767
C	-0.396391	-0.189446	-0.131449

N	-0.104657	-0.838923	1.213067
C	0.131900	1.276883	-0.039635
O	-0.546061	-0.285573	2.269081
H	-0.248593	-1.360978	-1.968043
H	1.277463	-0.549279	-1.514167
H	1.942088	-2.470309	-0.484770
H	0.330097	-3.222863	-0.624970
O	-0.619003	2.273786	-0.120090
N	1.448913	1.381995	0.117188
H	2.158913	0.555143	0.153354
H	0.819857	-2.499730	1.976877
O	3.481359	-0.532648	-1.263843
O	3.411696	-0.346109	0.062715
C	2.049277	2.696533	0.213333
H	3.130445	2.555564	0.289861
H	1.824057	3.307225	-0.670507
H	1.686079	3.244152	1.093104
C	-1.926688	-0.406371	-0.331753
O	-2.348618	-1.556242	-0.466494
N	-2.702197	0.695568	-0.360983
H	-2.201272	1.581668	-0.220081
C	-4.137704	0.618148	-0.500278
H	-4.650859	0.758068	0.462324
H	-4.495806	1.387338	-1.195533
H	-4.394768	-0.370775	-0.886308

DiMAPO-O₂ pos displacement

C	0.069889	-0.776258	-1.583993
C	0.789134	-2.089902	-1.194534
C	1.522232	-1.687858	0.082555
C	-0.336625	-0.117923	-0.223514
N	0.541570	-0.826439	0.726509
C	-0.018505	1.421199	-0.232236
O	0.418232	-0.724674	1.990712
H	-0.799425	-0.951368	-2.224037
H	0.764096	-0.113779	-2.105300
H	1.477276	-2.441567	-1.970457
H	0.060165	-2.871588	-0.963262
O	-0.932034	2.229212	-0.593698
N	1.226037	1.720398	0.063317
H	2.451065	0.656810	0.530430
H	1.782846	-2.480181	0.792870
O	2.683944	-0.986710	-0.362223
O	3.135489	-0.093472	0.687910
C	1.539705	3.134841	-0.033502
H	2.600429	3.285311	0.206179
H	1.352094	3.543723	-1.040323
H	0.940043	3.748258	0.659070
C	-1.799544	-0.552766	0.095115
O	-2.063120	-1.745002	0.274765
N	-2.714802	0.439626	0.086345
H	-2.325498	1.367794	-0.162694
C	-4.122251	0.190980	0.282764
H	-4.513285	0.763262	1.135472
H	-4.709181	0.465035	-0.606368

H -4.254546 -0.875520 0.479576

EMAPO-O₂ TS

C	-0.083964	-0.874226	-1.451336
C	0.487599	-2.250831	-1.044340
C	1.158153	-1.914205	0.251048
C	-0.360102	-0.153860	-0.103569
N	0.514329	-0.897121	0.847551
C	0.006631	1.362371	-0.126942
O	0.763058	-0.425524	2.020597
H	-0.974400	-0.928678	-2.079738
H	0.699464	-0.324191	-1.974165
H	1.206425	-2.623810	-1.780764
H	-0.305102	-3.007416	-0.921398
O	-0.888481	2.215610	-0.077090
N	1.315008	1.623768	-0.258549
H	2.083349	0.886701	-0.057374
H	1.654768	-2.616446	0.906202
O	2.777993	-1.187712	-0.516053
O	3.229566	-0.147951	0.229027
C	1.743865	3.006191	-0.252485
H	1.284832	3.570686	-1.074354
H	1.477247	3.518209	0.683243
H	2.831944	3.022143	-0.369577
C	-1.823316	-0.255227	0.353347
O	-2.218389	-0.507237	1.466664
C	-4.047806	0.056825	-0.324285
H	-4.590384	0.239263	-1.254553
H	-4.395469	-0.868951	0.145594
H	-4.202178	0.885091	0.373833
O	-2.671524	-0.034855	-0.689218

EMAPO-O₂ neg displacement

C	0.233499	-1.003524	-1.124411
C	0.747153	-2.334445	-0.512767
C	0.636948	-2.105954	0.953318
C	-0.396434	-0.212576	0.051031
N	0.043988	-0.986777	1.280239
C	0.075613	1.263106	0.225951
O	-0.170196	-0.513332	2.433874
H	-0.499055	-1.164708	-1.918316
H	1.097869	-0.475396	-1.546554
H	1.786595	-2.496088	-0.819201
H	0.155912	-3.207381	-0.833763
O	-0.754526	2.155273	0.428979
N	1.398613	1.440821	0.142783
H	2.114235	0.650031	-0.005606
H	1.012599	-2.732047	1.752666
O	3.207612	-0.540751	-1.639791
O	3.364519	-0.292746	-0.331954
C	1.947703	2.764271	0.342650
H	1.538890	3.481935	-0.380778
H	1.725917	3.149073	1.347468
H	3.031141	2.696966	0.210705
C	-1.926028	-0.221993	-0.001988

O -2.682657 -0.703742 0.808036
C -3.762094 0.481846 -1.281636
H -3.931976 0.946897 -2.254751
H -4.262246 -0.490694 -1.229965
H -4.149373 1.121014 -0.482572
O -2.346861 0.340011 -1.163316

EMAPO-O₂ pos displacement

C -0.079786 -0.861356 -1.478247
C 0.645767 -2.181702 -1.124554
C 1.502609 -1.753652 0.062738
C -0.337367 -0.153394 -0.116117
N 0.587714 -0.876942 0.784617
C -0.032715 1.401604 -0.173730
O 0.747162 -0.598219 2.018248
H -1.002193 -1.016404 -2.038229
H 0.591873 -0.232236 -2.064852
H 1.254187 -2.562280 -1.950938
H -0.058828 -2.964463 -0.815937
O -1.023645 2.162378 -0.261980
N 1.255542 1.687007 -0.159155
H 2.475415 0.644921 0.235225
H 1.837144 -2.528084 0.762976
O 2.613609 -1.079323 -0.529037
O 3.162548 -0.113648 0.401316
C 1.544380 3.106371 -0.252845
H 1.116181 3.569344 -1.158187
H 1.140305 3.679007 0.599375
H 2.632699 3.252964 -0.275722
C -1.777129 -0.287996 0.391517
O -2.126101 -0.407972 1.542867
C -4.030419 -0.108870 -0.229904
H -4.615406 -0.078198 -1.152183
H -4.346903 -0.950560 0.394954
H -4.161601 0.819762 0.333555
O -2.670786 -0.247000 -0.636591

N 0.822783 0.747679 -0.515050
C -0.785633 1.394071 1.242241
C -1.345017 -0.567981 -0.317095
O 0.578033 1.782031 -1.211018
H 1.056169 -0.221665 2.195098
H 0.073484 -1.605711 1.653696
H 1.545049 -2.067916 -0.170229
H 2.759244 -1.344210 0.929316
H 2.669284 0.236662 -1.271223
H -0.008945 1.909078 1.825688
H -1.236954 2.097292 0.541105
H -1.571798 1.032591 1.909413
O -2.520907 -0.149502 -0.156092
N -0.866692 -1.594117 -0.993979
H -1.682217 -2.034287 -1.440077

AMPO-NH-b

C 0.440392 -1.444616 0.639258
C 1.508680 -1.515387 -0.478291
C 1.881655 -0.074757 -0.638648
C -0.158368 -0.038931 0.509297
N 1.002725 0.725530 -0.084319
C -0.583850 0.605038 1.820824
C -1.447325 -0.070133 -0.494346
O 1.034533 1.999568 -0.069109
H 0.925366 -1.573957 1.618611
H -0.366454 -2.170421 0.525420
H 1.079814 -1.925046 -1.406878
H 2.364487 -2.152326 -0.213274
H 2.700442 0.356745 -1.201393
H 0.204984 0.553375 2.586401
H -0.840785 1.653616 1.651272
H -1.469663 0.074942 2.184962
O -2.139234 -1.108065 -0.314304
N -1.670535 0.938399 -1.295156
H -0.933024 1.636268 -1.170057

AMPO-OOH cis 2-a

C 0.763146 1.740561 0.327633
C -0.585781 1.860561 -0.410157
C -1.444942 0.735540 0.165482
C 0.969545 0.230450 0.528234
N -0.432587 -0.236335 0.655979
C 1.778287 -0.149576 1.775377
C 1.657565 -0.395207 -0.730894
O -0.752491 -1.456548 0.899947
H 0.715115 2.236006 1.303792
H 1.589695 2.163924 -0.244258
H -0.452198 1.674382 -1.481387
H -1.060198 2.836883 -0.289781
H 1.356426 0.332931 2.662963
H 1.767134 -1.231979 1.927132
H 2.815597 0.177412 1.654428
O 2.395572 0.272391 -1.441430

B3LYP/6-31G*

Scheme 2 Structures

Hydroperoxyl Radical

O 0.055881 0.719946 0.000000
O 0.055881 -0.611439 0.000000
H -0.894102 -0.868053 0.000000

AMPO-NH-a

C 0.656250 -0.746501 1.314314
C 1.821360 -1.161841 0.383412
C 1.901975 0.008627 -0.541053
C -0.207762 0.217459 0.472729

N	1.425219	-1.720046	-0.903792
H	1.799847	-2.160054	-1.733103
H	0.695094	-2.183364	-0.374584
H	-2.089046	1.025338	1.003416
O	-2.231224	0.161639	-0.846215
O	-3.201699	-0.714888	-0.206933
H	-2.594061	-1.411531	0.129067

AMPO-OOH trans-2

C	0.362154	1.611760	0.562466
C	-0.646665	1.791308	-0.592360
C	-1.384544	0.457485	-0.681768
C	0.770003	0.128663	0.522849
N	-0.391245	-0.497692	-0.162591
C	0.987546	-0.498869	1.907141
C	2.057600	-0.081801	-0.334878
O	-0.622805	-1.760816	-0.140598
H	-0.120273	1.829703	1.520259
H	1.242287	2.247731	0.456230
H	-0.125243	1.970401	-1.538598
H	-1.346951	2.613561	-0.428231
H	-1.699697	0.144502	-1.681078
H	0.108013	-0.332586	2.536983
H	1.161151	-1.574467	1.825639
H	1.857418	-0.036316	2.383694
O	2.894709	0.799997	-0.460951
N	2.179085	-1.326841	-0.861860
H	2.989856	-1.532018	-1.428552
H	1.428080	-2.002663	-0.791101
O	-2.512148	0.480710	0.174801
O	-3.288470	-0.718472	-0.093918
H	-2.656369	-1.418750	0.180541

AMPO-OOH cis-2b

C	-0.459528	-1.484446	-1.068178
C	1.036953	-1.157406	-1.245048
C	1.539871	-0.780081	0.153549
C	-0.930386	-0.575357	0.075784
N	0.305694	-0.454731	0.889231
C	-2.069370	-1.155965	0.922102
C	-1.354292	0.826899	-0.467560
O	0.333198	0.065033	2.053360
H	-0.596477	-2.532177	-0.778275
H	-1.036924	-1.290232	-1.973223
H	1.150309	-0.287941	-1.897554
H	1.607854	-1.986396	-1.671171
H	-1.811755	-2.164252	1.262939
H	-2.257417	-0.530008	1.797540
H	-2.984167	-1.208907	0.323427
O	-1.721590	0.980873	-1.624314
N	-1.349457	1.811182	0.469787
H	-1.494832	2.756324	0.141003
H	-0.824916	1.674326	1.327725
H	2.067662	-1.587876	0.676542

O	2.500137	0.254964	0.224127
O	1.930416	1.452798	-0.383292
H	2.570232	1.590768	-1.105026

AMPO-OOH cis-3

C	0.504640	-0.878971	1.514047
C	-0.997420	-0.535064	1.623850
C	-1.575700	-0.742491	0.217018
C	0.897581	-0.542036	0.053153
N	-0.378460	-0.767690	-0.646313
C	1.972588	-1.464329	-0.539392
C	1.298560	0.953963	-0.109510
O	-0.450907	-0.942351	-1.905384
H	0.669273	-1.950610	1.675841
H	1.109692	-0.336555	2.246439
H	-1.142975	0.514145	1.889219
H	-1.509305	-1.152982	2.365568
H	1.634076	-2.502956	-0.479121
H	2.145394	-1.222641	-1.590893
H	2.919123	-1.387210	0.005972
O	0.585531	1.780939	-0.666376
N	2.495254	1.304150	0.436328
H	2.808409	2.257313	0.310673
H	3.150741	0.629145	0.797723
H	-2.117096	-1.686308	0.081583
O	-2.531829	0.199463	-0.216595
O	-2.075491	1.549037	0.058596
H	-1.304809	1.640306	-0.550026

AMPO-O2 cis-1

C	-0.378686	-1.129497	-1.279977
C	1.057935	-1.650845	-1.019275
C	1.590397	-0.670008	0.026413
C	-0.852533	-0.469076	0.054461
N	0.402843	-0.445338	0.840056
C	-1.903497	-1.298149	0.795474
C	-1.418637	0.969635	-0.241922
O	0.453053	-0.300794	2.108847
H	-1.056753	-1.932740	-1.588175
H	-0.361218	-0.382334	-2.076327
H	1.676686	-1.663032	-1.922803
H	1.047652	-2.661945	-0.592733
H	-1.626626	-2.360961	0.830242
H	-1.997896	-0.934079	1.822689
H	-2.857986	-1.173295	0.280137
O	-2.596360	1.007073	-0.675734
N	-0.563329	1.961049	-0.046123
H	-1.027202	2.827169	-0.331493
H	1.036086	1.849846	0.151623
H	2.382497	-1.025035	0.696863
O	2.005905	0.468957	-0.712733
O	2.054688	1.616524	0.174797

AMPO-O2 trans-2

C	0.271756	1.725507	0.283343
C	-0.936331	1.814875	-0.689061
C	-1.484305	0.389637	-0.743984
C	0.630158	0.223482	0.377372
N	-0.280502	-0.402376	-0.632278
C	0.417888	-0.367214	1.786625
C	2.081561	-0.065661	-0.081262
O	-0.395742	-1.734161	-0.631728
H	-0.007028	2.102064	1.272840
H	1.135275	2.302626	-0.057265
H	-0.620312	2.127246	-1.691068
H	-1.704364	2.513609	-0.341225
H	-2.033692	0.094174	-1.646372
H	-0.557184	-0.051682	2.166635
H	0.419208	-1.457967	1.719218
H	1.208996	-0.040120	2.474526
O	2.970540	0.786721	-0.123953
N	2.276258	-1.378561	-0.392318
H	3.131022	-1.591198	-0.891118
H	1.402968	-1.902962	-0.591311
O	-2.355921	0.216528	0.373165
O	-2.997571	-1.013213	0.277406

AMPO-O2 cis-1b

C	0.597542	-0.631218	1.581895
C	-0.914581	-0.331331	1.648720
C	-1.476784	-0.778209	0.289008
C	0.973132	-0.447864	0.093077
N	-0.280691	-0.881851	-0.558922
C	2.136320	-1.321107	-0.368061
C	1.322014	1.069274	-0.164607
O	-0.346330	-1.383436	-1.732130
H	0.796109	-1.669372	1.886648
H	1.197583	0.028032	2.215879
H	-1.100104	0.740965	1.734864
H	-1.416253	-0.841312	2.478450
H	1.995699	-2.366028	-0.062036
H	2.208516	-1.292385	-1.459195
H	3.057028	-0.921868	0.061962
O	2.456869	1.435073	0.225395
N	0.356442	1.781188	-0.726174
H	0.688299	2.747486	-0.792907
H	-1.218490	1.528315	-0.524944
H	-1.956796	-1.767229	0.306694
O	-2.497747	0.024415	-0.265737
O	-2.188754	1.444045	-0.143770

H2O

O	0.000000	0.000000	0.119738
H	0.000000	0.761560	-0.478953
H	0.000000	-0.761560	-0.478953

Hydroxide ion

O	0.000000	0.000000	0.109707
H	0.000000	0.000000	-0.877653

Peroxide

O	0.056561	0.815957	0.000000
O	0.056561	-0.710399	0.000000
H	-0.904975	-0.844464	0.000000

Restricted AMPO-O₂-A

C	0.019089	1.302677	-1.183099
C	-1.433727	1.372074	-0.637756
C	-1.442419	0.435727	0.568147
C	0.856649	0.590465	-0.092913
N	-0.100235	0.497639	1.039151
C	2.090386	1.381124	0.372246
C	1.334994	-0.807875	-0.590584
O	0.234563	-0.167605	2.149793
H	0.417574	2.304264	-1.384482
H	0.085536	0.730710	-2.110883
H	-2.184579	1.014015	-1.347700
H	-1.699182	2.390933	-0.330098
H	1.802154	2.410177	0.620067
H	2.501950	0.911762	1.270805
H	2.858173	1.403179	-0.410156
O	1.556150	-1.045918	-1.778201
N	1.551794	-1.702186	0.414628
H	1.616265	-2.664677	0.115372
H	1.069754	-1.468118	1.303613
H	-2.158826	0.700898	1.357039
O	-1.728864	-0.936477	0.158762
O	-2.939295	-0.968309	-0.514889

Restricted AMPO-O₂-B

C	-0.370294	-1.224780	-1.232329
C	1.069648	-1.720150	-0.936819
C	1.598476	-0.656292	0.031895
C	-0.843561	-0.490301	0.064931
N	0.394618	-0.465371	0.869334
C	-1.934823	-1.249706	0.825713
C	-1.370412	0.932744	-0.289880
O	0.408045	-0.148749	2.107159
H	-1.053431	-2.042672	-1.488628
H	-0.353097	-0.528168	-2.073230
H	1.682042	-1.776599	-1.842421
H	1.063316	-2.706106	-0.454336
H	-1.668132	-2.309230	0.925878
H	-2.039326	-0.825580	1.828720
H	-2.882083	-1.153912	0.290368
O	-2.519364	1.049324	-0.741552
N	-0.518903	1.951690	-0.092130
H	-0.865060	2.840077	-0.425365
H	0.497547	1.864531	0.099383

H	2.409228	-0.947351	0.716632
O	1.912836	0.449533	-0.741803
O	2.096581	1.603853	0.151385

H	2.958868	-0.092833	1.419544
H	3.162352	-1.136456	0.015303
N	2.157838	0.674349	-0.360051
H	0.949179	2.286396	-1.568508

OH radical

O	0.000000	0.000000	0.109213
H	0.000000	0.000000	-0.873700

B3LYP/6-31G*

IMIC acids and Lactims

lactim-1 TAMPO

C	0.732488	-0.602221	1.442063
C	2.151691	-0.779977	0.843345
C	2.193752	0.270518	-0.221771
C	-0.076287	0.159785	0.370653
N	1.025762	0.828464	-0.447000
C	-1.157538	1.139680	0.821643
C	-0.902998	-0.754681	-0.543900
O	0.730553	1.736109	-1.271315
H	0.785422	0.009935	2.347758
H	0.265305	-1.553564	1.708977
H	2.299672	-1.789225	0.431866
H	2.935768	-0.637717	1.596584
H	3.051531	0.615889	-0.784407
H	-1.037246	1.462516	1.859605
H	-1.095041	2.014873	0.166930
O	-0.297237	-1.660447	-1.344194
C	-2.472714	0.357797	0.555710
H	-2.858983	-0.116315	1.468036
H	-3.269859	1.002101	0.170442
N	-2.164623	-0.683121	-0.430561
H	0.618567	-1.376582	-1.505256

lactim-2 TAMPO

C	-0.849119	0.529462	1.444978
C	-2.225534	0.711469	0.757670
C	-2.190266	-0.323803	-0.318769
C	0.041265	-0.156626	0.389878
N	-0.994411	-0.810059	-0.526596
C	1.107453	-1.164135	0.841180
C	0.895869	0.802285	-0.422837
O	-0.616667	-1.663044	-1.379109
H	-0.948682	-0.134106	2.310063
H	-0.423068	1.473767	1.794106
H	-2.335007	1.719881	0.334326
H	-3.057420	0.565215	1.456698
H	-3.004559	-0.658143	-0.948054
H	1.005501	-1.439336	1.894634
H	0.985106	-2.060109	0.225177
O	0.259198	1.765573	-1.118101
C	2.457580	-0.464410	0.516388

imic acid-1 MAMPO

C	0.810937	-1.575110	0.143999
C	2.233352	-1.385705	-0.448592
C	2.265229	0.062674	-0.808702
C	0.294904	-0.158460	0.460963
N	1.250145	0.722775	-0.336429
C	0.437817	0.246258	1.938026
C	-1.146099	0.100886	-0.003999
O	1.026574	1.988162	-0.422513
H	0.816136	-2.202179	1.038296
H	0.139164	-2.042182	-0.577324
H	2.410712	-2.030149	-1.317642
H	3.024626	-1.621082	0.277962
H	1.457672	0.058496	2.291584
H	0.208879	1.306256	2.070765
H	-0.258860	-0.344929	2.539344
O	-1.492631	1.398276	-0.136419
N	-1.934769	-0.884584	-0.137461
C	-3.322958	-0.613069	-0.488469
H	3.028811	0.600472	-1.356996
H	-3.449000	0.285984	-1.104228
H	-3.921701	-0.479057	0.422842
H	-3.728669	-1.477917	-1.023203
H	-0.646040	1.922599	-0.232075

imic acid-2 MAMPO

C	-0.831750	1.493530	0.639387
C	-1.847070	1.640161	-0.527422
C	-2.094443	0.231550	-0.956438
C	-0.332192	0.037455	0.592561
N	-1.296719	-0.619635	-0.383638
C	-0.421651	-0.700601	1.934505
C	1.080033	-0.126453	0.003920
O	-1.214037	-1.889603	-0.578357
H	-1.329047	1.679221	1.595682
H	0.015218	2.173960	0.550242
H	-1.436225	2.227476	-1.360677
H	-2.769804	2.144697	-0.217001
H	-1.440629	-0.648633	2.332234
H	-0.141666	-1.750151	1.824913
H	0.259757	-0.224093	2.645777
O	1.379460	-1.369234	-0.435767
N	1.893205	0.847441	0.024377
C	3.244057	0.620222	-0.475352
H	-2.799708	-0.128172	-1.695545
H	3.274043	-0.045359	-1.347239
H	3.869000	0.166554	0.305994
H	3.690569	1.583244	-0.741254
H	0.527815	-1.877867	-0.532279

	C	1.727192	-1.764321	-0.474371
imic-acid-3 MAMPO	C	2.273776	-0.378947	-0.470727
	C	0.064813	-0.107684	0.331507
	N	1.415167	0.504196	-0.055627
	C	-0.009133	-0.033034	1.865314
	C	-1.116442	0.698342	-0.290373
	O	1.624930	1.759463	0.126722
	H	-0.207372	-2.288203	0.437117
	H	-0.326898	-1.615369	-1.187670
	H	1.928104	-2.289881	-1.414968
	H	2.186432	-2.366573	0.323012
	H	0.789975	-0.628635	2.321585
	H	0.099966	1.005247	2.189266
	H	-0.973294	-0.409496	2.215825
	O	-0.834400	1.962141	-0.654044
	N	-2.309251	0.294830	-0.442726
	C	-2.813432	-1.006964	-0.073214
	H	3.276973	-0.053823	-0.715818
	H	-2.241245	-1.561484	0.685712
	H	-2.898328	-1.651442	-0.959754
	H	-3.830382	-0.881874	0.317252
	H	0.101702	2.176862	-0.394531
imic acid-7 MAMPO	C	0.878512	-1.354285	-0.880276
	C	1.660180	-0.202697	-1.557110
	C	1.810010	0.774311	-0.436920
	C	0.122533	-0.677653	0.291472
	N	1.012837	0.521004	0.568381
	C	0.064887	-1.501825	1.583701
	C	-1.289922	-0.235843	-0.176945
	O	0.900908	1.142806	1.667249
	H	1.582155	-2.091562	-0.478098
	H	0.203099	-1.868024	-1.568226
	H	1.101438	0.229423	-2.400589
	H	2.625418	-0.536209	-1.954497
	H	1.078911	-1.768644	1.897350
	H	-0.400125	-0.917066	2.379527
	H	-0.496542	-2.432897	1.451359
	O	-2.088432	-1.335736	-0.431563
	N	-1.823867	0.873539	-0.432333
	C	-1.245332	2.196424	-0.293766
	H	2.467763	1.631637	-0.377896
	H	-0.623876	2.324281	0.597918
	H	-2.067779	2.918227	-0.254848
	H	-0.647241	2.447111	-1.180826
	H	-1.651025	-2.145223	-0.129948
imic acid 8 MAMPO	C	-0.308525	1.599803	0.252976
	C	-1.528035	1.662823	-0.698574
	C	-2.216397	0.368011	-0.418373
	C	-0.058183	0.088559	0.472171
	N	-1.452282	-0.490070	0.208530
imic acid-6 MAMPO	C	0.211347	-1.540948	-0.239800

C 0.330470 -0.325622 1.892155
 C 0.926829 -0.465391 -0.576485
 O -1.718556 -1.664372 0.583907
 H -0.563334 2.060180 1.213649
 H 0.564338 2.117956 -0.149375
 H -1.216283 1.736658 -1.751774
 H -2.162257 2.533303 -0.494796
 H -0.393705 0.083324 2.604265
 H 0.308004 -1.414590 1.971289
 H 1.323135 0.038418 2.159810
 O 0.302174 -1.213390 -1.520104
 N 2.178970 -0.289584 -0.686222
 C 2.994230 0.507357 0.207452
 H -3.216256 0.066599 -0.700628
 H 2.463493 1.286965 0.770473
 H 3.774585 0.998763 -0.384506
 H 3.505973 -0.141614 0.930556
 H 1.014221 -1.499526 -2.123468

imic acid-1 diMAPO

C -0.330407 0.872822 1.664887
 C -1.259123 2.039684 1.259584
 C -0.817316 2.320800 -0.138556
 C 0.005853 0.191227 0.311463
 N -0.121557 1.347567 -0.654199
 C 1.403872 -0.454843 0.350477
 O 1.589362 -1.343765 1.200283
 C 3.666434 -0.572501 -0.572738
 H -0.786555 0.170818 2.364581
 H 0.587468 1.258254 2.119947
 H -1.150377 2.907616 1.918883
 H -2.316213 1.740735 1.278955
 H 3.850825 -1.143437 0.337813
 H 4.405190 0.230068 -0.658942
 C -1.065802 -0.873215 -0.011205
 O -0.912510 -2.043781 0.650514
 C -3.066784 -1.603684 -0.971542
 H -3.599300 -1.379487 -1.900500
 H -2.657325 -2.620017 -1.026008
 H -1.038367 3.183022 -0.753882
 O 0.377043 1.278470 -1.831217
 H -3.799317 -1.586555 -0.152772
 N -2.045409 -0.585636 -0.758059
 N 2.328677 -0.005966 -0.504202
 H 1.967954 0.592860 -1.255890
 H 3.766720 -1.239654 -1.437163
 H -0.014197 -2.055113 1.069358

imic acid-2 diMAPO

C 0.247225 1.494992 -1.273553
 C -0.688596 2.648179 -0.827193
 C -0.967998 2.328606 0.603471
 C 0.068849 0.391886 -0.219389
 N -0.564634 1.141970 0.938914

C -0.922540 -0.720920 -0.722830
 O -0.999020 -0.963116 -1.919475
 C -2.540660 -2.444702 -0.046809
 H 1.290995 1.810394 -1.278689
 H 0.004110 1.099949 -2.259204
 H -1.626375 2.673051 -1.400560
 H -0.225789 3.634948 -0.941811
 H -2.515125 -2.628066 -1.121450
 H -3.562176 -2.178868 0.249392
 C 1.384452 -0.274341 0.225251
 O 1.377279 -0.865586 1.440358
 C 3.578254 -0.977253 -0.219275
 H 4.430282 -0.426546 -0.631662
 H 3.709812 -1.094007 0.863096
 H -1.475400 2.934691 1.344341
 O -0.707792 0.565930 2.097147
 H 3.586349 -1.976324 -0.674438
 N 2.351235 -0.288350 -0.592717
 N -1.615543 -1.362768 0.245613
 H -1.511563 -1.029432 1.199800
 H -2.246258 -3.358043 0.482199
 H 0.626085 -0.474229 1.964054

imic acid-3 diMAPO

C -0.253051 -0.758567 1.676543
 C -1.590608 -1.529575 1.567127
 C -1.558758 -2.007959 0.151704
 C 0.005118 -0.286250 0.222209
 N -0.682719 -1.371577 -0.564328
 C -0.714244 1.064409 -0.009937
 O -0.061267 2.127138 0.503642
 C -2.540343 2.368738 -0.681273
 H 0.550134 -1.431492 1.992016
 H -0.285768 0.083249 2.369529
 H -2.454303 -0.871617 1.732301
 H -1.661189 -2.354283 2.284117
 H -1.858415 3.227129 -0.707166
 H -3.235788 2.514313 0.156400
 C 1.494637 -0.188233 -0.141510
 O 1.974760 -0.969939 -1.104292
 C 3.600893 0.800122 0.204275
 H 3.980688 1.708816 0.677762
 H 4.176415 -0.052062 0.587652
 H -2.165590 -2.770653 -0.318641
 O -0.397626 -1.548246 -1.810518
 H 3.774983 0.855255 -0.877474
 N 2.184643 0.654372 0.528374
 N -1.863328 1.086085 -0.540631
 H -3.135707 2.351476 -1.599835
 H 1.177925 -1.336354 -1.615179
 H 0.877641 1.846325 0.709130

imic acid-4 diMAPO

C 0.179795 0.804174 -1.661954

C	0.851328	2.198125	-1.531008	N	0.753548	0.899707	-0.088060
C	0.738009	2.513126	-0.077743	C	-0.493498	0.118578	1.903739
C	0.018618	0.276323	-0.225265	C	-1.383730	-0.345130	-0.396941
N	0.305382	1.509915	0.616042	O	0.293511	2.098063	-0.034414
C	-1.402370	-0.248525	0.088120	H	1.237789	-1.694441	1.366985
O	-1.785135	-0.240903	1.384539	H	0.392849	-2.328359	-0.039563
C	-3.402786	-1.272455	-0.579300	H	2.014991	-1.424211	-1.531626
H	0.777581	0.099281	-2.237952	H	3.029961	-1.259710	-0.104401
H	-0.806608	0.876744	-2.119228	H	2.538967	1.231152	-1.049816
H	0.364259	2.960903	-2.149506	H	0.396933	0.256294	2.526215
H	1.909395	2.183671	-1.827848	H	-1.081114	1.038374	1.922633
H	-3.880798	-0.840511	0.308271	H	-1.096257	-0.693350	2.321625
H	-3.309982	-2.354787	-0.419444	O	-1.910569	0.833923	-0.762382
C	1.067440	-0.793169	0.169533	N	-2.004818	-1.415594	-0.690174
O	1.292184	-0.950657	1.495414	H	-1.522312	-2.237419	-0.328453
C	2.559501	-2.523464	-0.352499	H	-1.277866	1.562782	-0.530462
H	3.279681	-2.665573	-1.164276				
H	3.097364	-2.304283	0.577921				
H	1.005676	3.428309	0.437195				
O	0.164689	1.447364	1.914444				
H	2.024737	-3.472573	-0.215931				
N	1.616695	-1.482346	-0.738661				
N	-2.091506	-0.708825	-0.868623				
H	-4.050051	-1.124375	-1.449560				
H	0.936189	-0.167180	1.980910				
H	-1.192544	0.377933	1.883657				

imic acid-1 AMPO

C	0.477776	-1.545393	0.373352
C	1.670202	-1.398635	-0.604817
C	1.952324	0.065411	-0.555988
C	-0.150362	-0.132584	0.477363
N	0.996763	0.751891	0.012099
C	-0.547076	0.290057	1.895472
C	-1.340689	0.089317	-0.486483
O	0.910075	2.010546	0.160285
H	0.841233	-1.849356	1.360061
H	-0.229632	-2.305568	0.031896
H	1.404221	-1.717336	-1.623403
H	2.529544	-2.006027	-0.298698
H	2.798935	0.596891	-0.970503
H	0.274022	0.104880	2.595807
H	-0.784709	1.355871	1.902153
H	-1.424734	-0.270710	2.233649
O	-2.312317	-0.872155	-0.402774
N	-1.526469	1.043553	-1.291145
H	-0.762360	1.718870	-1.221898
H	-2.093692	-1.511773	0.290769

imic acid-2 AMPO

C	0.875881	-1.438334	0.367278
C	2.058561	-0.978895	-0.527848
C	1.879693	0.499565	-0.600014
C	-0.093339	-0.238416	0.465264

N	0.753548	0.899707	-0.088060
C	-0.493498	0.118578	1.903739
C	-1.383730	-0.345130	-0.396941
O	0.293511	2.098063	-0.034414
H	1.237789	-1.694441	1.366985
H	0.392849	-2.328359	-0.039563
H	2.014991	-1.424211	-1.531626
H	3.029961	-1.259710	-0.104401
H	2.538967	1.231152	-1.049816
H	0.396933	0.256294	2.526215
H	-1.081114	1.038374	1.922633
H	-1.096257	-0.693350	2.321625
O	-1.910569	0.833923	-0.762382
N	-2.004818	-1.415594	-0.690174
H	-1.522312	-2.237419	-0.328453
H	-1.277866	1.562782	-0.530462

imic acid-3 AMPO

C	0.910669	-1.400492	0.441046
C	2.068570	-0.956852	-0.494771
C	1.851162	0.512233	-0.649311
C	-0.070765	-0.214199	0.498275
N	0.724159	0.913671	-0.141581
C	-0.463245	0.209711	1.919269
C	-1.339884	-0.406178	-0.350347
O	0.217186	2.096973	-0.161271
H	1.295901	-1.604041	1.444279
H	0.395097	-2.290974	0.081403
H	2.022640	-1.455667	-1.473064
H	3.055356	-1.185793	-0.075191
H	2.480628	1.231273	-1.158950
H	0.432316	0.404568	2.518404
H	-1.077792	1.112014	1.904048
H	-1.031946	-0.600111	2.385835
O	-1.984360	0.728291	-0.689486
N	-1.747920	-1.578927	-0.622729
H	-2.629082	-1.522450	-1.142770
H	-1.378450	1.500530	-0.512729

imic acid-4 AMPO

C	0.911230	-1.399237	0.444382
C	2.066781	-0.957865	-0.495308
C	1.850488	0.511407	-0.650188
C	-0.070782	-0.213332	0.499233
N	0.724128	0.913674	-0.141631
C	-0.464709	0.212044	1.919315
C	-1.338917	-0.406879	-0.350530
O	0.217344	2.097136	-0.161980
H	1.298845	-1.598397	1.447601
H	0.395680	-2.291486	0.089129
H	2.016821	-1.457180	-1.473167
H	3.054570	-1.187950	-0.078802
H	2.479672	1.229841	-1.161019
H	0.430206	0.408923	2.518733

H	-1.080552	1.113434	1.902574
H	-1.032566	-0.597998	2.386557
O	-1.983402	0.727073	-0.691641
N	-1.746146	-1.580080	-0.622086
H	-2.626738	-1.524577	-1.143215
H	-1.377899	1.499727	-0.514828

imic acid-5 AMPO

C	0.980309	-0.934121	1.054332
C	2.031980	-0.986075	-0.080357
C	1.804256	0.304820	-0.795845
C	-0.096724	0.054000	0.573644
N	0.682025	0.891738	-0.465599
C	-0.638321	0.999882	1.641372
C	-1.210849	-0.641579	-0.211596
O	0.188444	1.970331	-0.897559
H	1.438280	-0.535454	1.965314
H	0.557932	-1.914619	1.274204
H	1.857818	-1.845499	-0.741499
H	3.054014	-1.073631	0.307499
H	2.426837	0.769522	-1.549608
H	0.193575	1.452409	2.190013
H	-1.227085	1.791961	1.177582
H	-1.266671	0.451389	2.350698
O	-2.284425	0.172881	-0.383211
N	-1.064440	-1.832916	-0.634590
H	-1.877124	-2.163535	-1.164662
H	-2.936728	-0.271558	-0.951361

imic acid-6 AMPO

C	0.980334	-0.934408	1.054063
C	2.031661	-0.986394	-0.080928
C	1.804145	0.304801	-0.795959
C	-0.096690	0.053862	0.573710
N	0.682109	0.891882	-0.465323
C	-0.638314	0.999465	1.641667
C	-1.210867	-0.641468	-0.211671
O	0.188766	1.970783	-0.896765
H	1.438616	-0.535801	1.964916
H	0.557916	-1.914867	1.274029
H	1.856986	-1.845570	-0.742263
H	3.053777	-1.074422	0.306596
H	2.426753	0.769639	-1.549615
H	0.193543	1.451799	2.190527
H	-1.226977	1.791704	1.178008
H	-1.266781	0.450820	2.350769
O	-2.283911	0.173523	-0.384048
N	-1.065002	-1.833102	-0.634023
H	-1.877714	-2.163510	-1.164186
H	-2.936318	-0.270844	-0.952137

imic acid-7 AMPO

C	0.769514	-0.714708	1.303063
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C	1.962984	-1.007916	0.356787
C	1.870569	0.090950	-0.649050
C	-0.170948	0.228263	0.514871
N	0.743645	0.751334	-0.595729
C	-0.680794	1.425900	1.307144
C	-1.306622	-0.532460	-0.174091
O	0.332999	1.698982	-1.324755
H	1.120216	-0.194493	2.199699
H	0.260981	-1.626627	1.622674
H	1.862602	-1.990838	-0.122761
H	2.919869	-1.007077	0.892538
H	2.585089	0.348218	-1.420139
H	0.159287	1.942652	1.780554
H	-1.180043	2.133342	0.640523
H	-1.371208	1.101780	2.092571
O	-0.830348	-1.622263	-0.829337
N	-2.552046	-0.293015	-0.184977
H	-2.782666	0.561510	0.319217
H	-1.604741	-2.030622	-1.259546

imic acid-8 AMPO

C	0.559309	-1.513108	0.439721
C	1.716642	-1.365953	-0.580431
C	1.931816	0.111090	-0.623787
C	-0.116992	-0.125650	0.499088
N	0.966244	0.785774	-0.059502
C	-0.486689	0.340972	1.909829
C	-1.342384	0.012436	-0.416671
O	0.825596	2.047626	0.023050
H	0.966706	-1.749121	1.427800
H	-0.149302	-2.296737	0.171826
H	1.442512	-1.754372	-1.572702
H	2.614397	-1.912466	-0.268808
H	2.739281	0.655878	-1.095805
H	0.372556	0.239824	2.581206
H	-0.793884	1.388702	1.886021
H	-1.308718	-0.270351	2.293560
O	-2.135316	-1.090336	-0.324686
N	-1.688192	0.988619	-1.144491
H	-1.008764	1.750633	-1.070107
H	-2.913611	-0.889789	-0.878452

mPW1K/6-31+G** Hydroperoxy Adducts

AMPO-OOH

C	0.440142	1.573543	-0.889230
C	-1.042352	1.896242	-0.598773
C	-1.544190	0.684023	0.163035
C	0.869741	0.519560	0.155581
N	-0.366926	0.313898	0.932787

C	2.001778	0.975785	1.074966	H	1.678213	-1.402290	-1.766405
C	1.304830	-0.797965	-0.529190	H	2.858266	-2.535313	-1.062296
O	-0.410146	-0.373089	2.000577	H	0.846930	-1.443336	2.828211
H	1.064342	2.465316	-0.812333	H	-0.274934	-0.085974	2.616424
H	0.574430	1.166850	-1.891357	O	-2.040468	-1.262234	0.076436
H	-1.622987	2.062778	-1.507070	C	-3.253003	-1.308344	-0.709082
H	-1.144998	2.776649	0.040142	O	-0.512281	-0.156942	-1.753140
H	2.917147	1.095527	0.492579	C	-4.388689	-0.632816	0.026617
H	1.743401	1.933129	1.533651	H	-5.308648	-0.716730	-0.559296
H	2.176173	0.249399	1.871059	H	-4.556445	-1.104564	0.997521
O	1.955897	-0.790844	-1.556422	H	-4.175450	0.425208	0.189075
N	0.916876	-1.946534	0.105151	H	-0.819811	-1.741427	2.279911
H	1.378918	-2.788933	-0.204404	O	3.198364	0.383815	-1.060201
H	0.640928	-1.888111	1.079175	H	3.606023	-0.825929	0.524626
H	-2.390404	0.813312	0.839585	O	-1.362598	1.136620	0.337730
O	-1.833022	-0.281140	-0.833614	C	-0.888780	2.413178	-0.157022
O	-2.212808	-1.502674	-0.204949	C	-1.977992	3.436355	0.059949
H	-1.365658	-1.982622	-0.209662	H	-3.067867	-0.853285	-1.686187

DMPO-OOH

N	-0.021737	-0.478092	-0.443758
C	-1.014647	0.591172	-0.504248
C	-0.190775	1.835939	-0.224595
C	0.976387	1.338132	0.640259
C	1.288788	-0.081478	0.135906
O	-1.963948	0.425451	0.527084
O	-2.860945	-0.619332	0.137184
C	1.675034	-1.046042	1.249783
C	2.336692	-0.091300	-0.980825
O	-0.362369	-1.692174	-0.610528
H	0.666113	1.294073	1.687826
H	1.849791	1.990978	0.576669
H	0.164064	2.244339	-1.174710
H	-0.794602	2.600314	0.266192
H	-1.531710	0.562859	-1.467333
H	0.904399	-1.074620	2.023540
H	1.804399	-2.055725	0.855885
H	2.615210	-0.723780	1.704902
H	3.319852	0.163198	-0.575677
H	2.394746	-1.084329	-1.432908
H	2.092135	0.628715	-1.766573
H	-2.263011	-1.389478	0.080900

DEPMPO-OOH

C	1.041835	-2.216404	0.141694
C	2.130354	-1.755868	-0.836446
C	2.768693	-0.570954	-0.136702
C	0.488768	-0.923124	0.772306
N	1.664111	-0.044284	0.683379
C	0.026167	-1.055898	2.218314
P	-0.861216	-0.244113	-0.312324
O	1.743717	1.091566	1.245749
H	1.470881	-2.831664	0.940037
H	0.264985	-2.805132	-0.348473

H	1.678213	-1.402290	-1.766405
H	2.858266	-2.535313	-1.062296
H	0.846930	-1.443336	2.828211
H	-0.274934	-0.085974	2.616424
O	-2.040468	-1.262234	0.076436
C	-3.253003	-1.308344	-0.709082
O	-0.512281	-0.156942	-1.753140
C	-4.388689	-0.632816	0.026617
H	-5.308648	-0.716730	-0.559296
H	-4.556445	-1.104564	0.997521
H	-4.175450	0.425208	0.189075
H	-0.819811	-1.741427	2.279911
O	3.198364	0.383815	-1.060201
H	3.606023	-0.825929	0.524626
O	-1.362598	1.136620	0.337730
C	-0.888780	2.413178	-0.157022
C	-1.977992	3.436355	0.059949
H	-3.067867	-0.853285	-1.686187
H	-3.456800	-2.370037	-0.864744
H	0.016193	2.662790	0.400739
H	-0.638267	2.307379	-1.215359
H	-1.627790	4.418054	-0.270945
H	-2.875487	3.183448	-0.509497
H	-2.243336	3.506556	1.117409
O	4.036536	1.319388	-0.369608
H	3.382522	1.769485	0.196964

CPCOMPO-OOH pos

C	0.139213	-0.667817	-1.459510
C	1.521728	-1.252322	-1.109170
C	1.846640	-0.748710	0.290214
C	-0.558740	-0.409893	-0.103911
N	0.518800	-0.567869	0.871173
C	-1.785246	-1.259441	0.223315
C	-1.134221	1.015358	-0.032661
O	0.318055	-0.445043	2.113745
H	-0.452095	-1.347739	-2.076663
H	0.267182	0.266644	-2.006869
H	2.287950	-0.944025	-1.819951
H	1.486642	-2.344845	-1.086757
H	-1.772923	-2.238842	-0.257671
H	-1.828940	-1.392167	1.307744
O	-0.510780	2.043030	0.064021
C	-2.936398	-0.379621	-0.252702
H	-3.188093	-0.541006	-1.304721
H	-3.840568	-0.469810	0.348388
O	-2.467740	0.976452	-0.114534
H	2.401838	-1.450570	0.917101
O	2.633634	0.414360	0.361060
O	2.156349	1.367832	-0.590738
H	1.413401	1.799068	-0.120684

TAMPO-OOH pos

C	0.468707	-0.515343	-1.598848
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C	1.743207	-1.150051	-1.006768
C	1.722335	-0.803673	0.473971
C	-0.528016	-0.375748	-0.436298
N	0.286529	-0.713819	0.742185
C	-1.819512	-1.205510	-0.493779
C	-1.047133	1.062133	-0.214551
O	-0.205574	-0.746207	1.908447
H	0.046746	-1.123969	-2.400909
H	0.699289	0.471288	-2.003584
H	2.649157	-0.776264	-1.482276
H	1.716796	-2.238564	-1.107145
H	-2.097427	-1.349852	-1.540851
H	-1.695191	-2.184166	-0.028581
O	-0.363729	2.079536	-0.243765
C	-2.884045	-0.356235	0.214024
H	-3.865227	-0.444486	-0.258369
H	-2.970311	-0.620232	1.271757
N	-2.360354	0.991282	0.065810
H	2.136422	-1.563888	1.140493
O	2.426075	0.358227	0.846898
O	2.314972	1.356348	-0.169779
H	1.432888	1.760222	-0.008074
H	-2.843567	1.811004	0.400650

EMPO-OOH pos

C	0.548394	1.138357	1.493075
C	0.931682	-0.318194	1.788624
C	1.479005	-0.853069	0.474651
C	0.095292	1.148481	0.017180
N	0.856267	0.011946	-0.526301
C	0.420497	2.435808	-0.723288
O	1.119060	-0.116130	-1.762025
H	1.423039	1.787851	1.584490
H	-0.223625	1.521370	2.163018
H	0.055864	-0.905545	2.070952
H	1.676321	-0.408156	2.580576
H	1.487000	2.650260	-0.633542
H	0.171300	2.343829	-1.781080
H	-0.156865	3.256893	-0.297780
C	-1.415667	0.874519	-0.056623
O	-1.697591	-0.430973	-0.047193
C	-3.097294	-0.778171	-0.093064
C	-3.192884	-2.283935	-0.128944
O	-2.249758	1.748951	-0.069761
H	-3.589568	-0.351510	0.784810
H	-3.536355	-0.315739	-0.980181
H	-4.243224	-2.582449	-0.174161
H	-2.683639	-2.687492	-1.006703
H	-2.750511	-2.730050	0.764810
O	2.878053	-0.682866	0.450459
H	1.244764	-1.897755	0.252818
O	3.391495	-1.398115	-0.677754
H	2.987417	-0.914845	-1.423391

TFMPO-OOH neg

N	-0.594332	-0.480201	-0.254770
C	-1.576764	0.581507	-0.512989
C	-0.857188	1.843832	-0.072197
C	0.161521	1.374653	0.977325
C	0.557277	-0.055609	0.572058
O	-2.706406	0.388155	0.304220
O	-3.515319	-0.634714	-0.282607
C	0.770197	-1.005819	1.742489
C	1.806487	-0.045212	-0.324773
O	-0.923321	-1.700850	-0.376534
H	-0.305766	1.330153	1.963622
H	1.026058	2.036145	1.049219
H	-0.359247	2.291111	-0.933776
H	-1.569131	2.567122	0.326753
H	-1.883109	0.546830	-1.561361
H	-0.136147	-1.033766	2.349180
H	0.980616	-2.015385	1.389821
H	1.599957	-0.659134	2.360808
H	-2.943638	-1.419778	-0.187884
F	2.883029	0.384155	0.363181
F	2.094186	-1.259862	-0.806984
F	1.660777	0.779848	-1.381207

DiEtMPO-OOH pos (DEPO-OOH)

C	0.106037	0.389099	1.646182
C	0.609533	1.844307	1.741028
C	0.208422	2.454300	0.410905
C	0.054005	0.062899	0.125726
N	0.415801	1.337652	-0.495987
C	1.063429	-0.995829	-0.339417
O	0.797699	-1.926447	-1.057222
O	2.276602	-0.720615	0.139408
C	3.343326	-1.580353	-0.314130
C	4.631657	-1.055573	0.270492
H	-0.891792	0.297722	2.075499
H	0.760829	-0.304880	2.172082
H	1.697210	1.878891	1.830592
H	0.168949	2.380860	2.582562
H	3.349413	-1.567866	-1.406455
H	3.125991	-2.600954	0.011187
H	4.604499	-1.068351	1.362591
H	4.823758	-0.033218	-0.062070
H	5.463555	-1.683942	-0.057258
C	-1.361179	-0.340946	-0.308803
O	-2.053362	0.307988	-1.061710
O	-1.741231	-1.459489	0.289572
C	-3.048846	-1.964988	-0.060020
H	-3.792154	-1.209522	0.206623
H	-3.078977	-2.104814	-1.142855
C	-3.249895	-3.259026	0.688895
H	-4.231605	-3.672276	0.444450
H	-2.489458	-3.992001	0.411832
H	-3.205134	-3.100924	1.768869
H	0.777440	3.311198	0.046140

O -1.165759 2.762222 0.535352
O -1.660317 3.157532 -0.741690
H -1.902842 2.288531 -1.119512
O 0.767716 1.440639 -1.705898

CPPO-OOH neg

N -0.604859 -0.426513 -0.498744
C -1.679046 0.559086 -0.432401
C -0.934133 1.852823 -0.149891
C 0.335599 1.411824 0.592150
C 0.705729 0.051447 -0.018675
O -2.533730 0.270085 0.653177
O -3.369161 -0.828636 0.275001
C 1.384295 -0.922021 0.946081
C 1.729686 0.143215 -1.167539
O -0.854172 -1.650281 -0.739496
H 0.118232 1.290428 1.657123
H 1.145075 2.138668 0.495677
H -0.689920 2.331351 -1.102283
H -1.553191 2.542202 0.425742
H -2.262448 0.532814 -1.356956
H 0.925617 -0.913991 1.938373
H 1.275642 -1.930782 0.536268
H 1.590324 -0.732281 -1.808958
H 1.581809 1.032860 -1.786752
H -2.718053 -1.543495 0.140198
C 2.850465 -0.477033 0.941364
H 3.526017 -1.300906 1.183110
H 3.013709 0.294705 1.700062
C 3.104737 0.101785 -0.475040
H 3.806811 -0.511912 -1.044588
H 3.546907 1.099819 -0.411551

DiMAMPO-OOH pos

C -0.486735 2.116343 -0.024945
C -1.480477 1.487788 -1.005302
C -1.992368 0.271912 -0.255470
C 0.232372 0.916183 0.611937
N -0.903735 -0.030003 0.681869
C 0.795419 1.222267 1.995225
C 1.378022 0.470239 -0.367135
O -1.040455 -0.961808 1.537106
H -1.018751 2.657822 0.764106
H 0.216768 2.786447 -0.514365
H -0.965983 1.163119 -1.913699
H -2.292724 2.156755 -1.290121
H 0.001181 1.593337 2.646824
H 1.239270 0.347094 2.468964
H 1.562857 1.994386 1.903450
O 1.733029 1.273721 -1.225832
N 1.975138 -0.743498 -0.248924
C 1.781374 -1.732971 0.792493
H -2.907443 0.440431 0.323291
O -2.202648 -0.803377 -1.130120

O -2.969799 -1.797262 -0.439993
H 0.924037 -1.507070 1.418367
H 2.683082 -1.805359 1.413048
H 1.608340 -2.711341 0.332874
C 3.050241 -1.062991 -1.172721
H 3.066809 -0.330495 -1.975711
H 4.016880 -1.050414 -0.655866
H 2.889595 -2.063675 -1.584063
H -2.351842 -2.079355 0.258509

DiMAPO-OOH neg

C -0.151579 -0.579377 1.664417
C -1.320410 -1.525551 1.360814
C -2.000514 -0.949082 0.126183
C 0.292934 -0.060366 0.277079
N -0.990973 -0.040750 -0.428890
C 1.005230 1.291545 0.414488
O -1.237677 0.637063 -1.477716
H 0.669363 -1.063181 2.192660
H -0.483981 0.269993 2.266324
H -2.028915 -1.591860 2.187548
H -0.962180 -2.529167 1.127844
O 1.983465 1.354309 1.164691
N 0.520484 2.329124 -0.274460
H -0.207189 2.126448 -0.953384
H -2.277487 -1.679208 -0.638064
O -3.136895 -0.213212 0.505715
O -3.911979 0.051946 -0.668103
C 1.132061 3.639203 -0.217765
H 0.359685 4.403731 -0.311295
H 1.641052 3.750736 0.738858
H 1.865578 3.773035 -1.019067
C 1.193686 -1.140068 -0.403645
O 0.668695 -2.023969 -1.067625
N 2.507793 -1.048410 -0.141185
H 2.807991 -0.285541 0.457225
C 3.458366 -2.027966 -0.618673
H 4.349791 -1.526068 -0.999999
H 3.753873 -2.719426 0.176805
H 2.993096 -2.598526 -1.421678
H -3.325325 0.650160 -1.165117

EMAPO-OOH neg

C 0.339719 -1.032212 1.572596
C -0.185735 -2.363347 0.993578
C -0.955578 -1.953446 -0.246406
C 0.357547 -0.031919 0.394003
N -0.162384 -0.831666 -0.726508
C -0.538284 1.202682 0.685826
O -0.154609 -0.423528 -1.927804
H 1.332301 -1.151219 2.005282
H -0.317406 -0.635424 2.345708
H -0.821538 -2.901700 1.697633
H 0.635103 -3.017993 0.693032

O	-0.666857	1.620276	1.822003
N	-1.164241	1.730829	-0.397221
H	-0.797111	1.459925	-1.302772
H	-1.064241	-2.682227	-1.051049
O	-2.218786	-1.515215	0.218850
O	-2.962306	-1.001157	-0.883283
C	-1.829164	3.016582	-0.284769
H	-2.452411	3.020632	0.609025
H	-1.107397	3.835372	-0.204726
H	-2.455919	3.171414	-1.163376
C	1.753066	0.473813	0.012786
O	2.038457	1.635692	-0.139394
C	3.926758	-0.180948	-0.554039
H	4.472633	-1.118322	-0.633742
H	3.892292	0.328615	-1.517815
H	4.388469	0.474305	0.185840
O	2.603299	-0.542365	-0.140795
H	-2.741970	-0.054365	-0.835016

MAMPO-OOH neg

C	1.074266	-1.448139	-0.963993
C	2.346062	-0.612934	-0.703405
C	1.852765	0.567875	0.111277
C	0.072533	-1.077368	0.152103
N	0.803630	-0.044558	0.910500
C	-0.292730	-2.242167	1.071798
C	-1.235009	-0.501826	-0.445246
O	0.386346	0.437246	2.010244
H	1.288353	-2.518030	-0.947738
H	0.635799	-1.219192	-1.935079
H	2.832212	-0.286603	-1.623785
H	3.076250	-1.165859	-0.107370
H	0.615540	-2.710521	1.458878
H	-0.889839	-1.898178	1.918662
H	-0.863280	-2.983739	0.509572
O	-1.714972	-0.969143	-1.465473
N	-1.803648	0.518687	0.252403
C	-3.136524	0.979403	-0.088339
H	2.560439	1.070781	0.772247
O	1.316787	1.474120	-0.838280
O	0.729717	2.575137	-0.149546
H	-1.457119	0.672104	1.193609
H	-3.210535	1.092196	-1.169715
H	-3.314818	1.943520	0.388950
H	-3.907290	0.271284	0.233129
H	-0.196787	2.285380	-0.092417

water

O	0.000000	0.000000	0.115880
H	0.000000	0.765693	-0.463520
H	0.000000	-0.765693	-0.463520

hydroxide ion

O	0.000000	0.000000	0.107252
H	0.000000	0.000000	-0.858012

B3LYP/6-31G*

Hydroperoxy adducts

AMPO-OOH neg

C	0.480032	1.600563	-0.867969
C	-1.018596	1.925453	-0.609790
C	-1.541034	0.714194	0.155418
C	0.880122	0.515071	0.168387
N	-0.370729	0.335731	0.947989
C	2.027295	0.927233	1.101757
C	1.283524	-0.810795	-0.539808
O	-0.438691	-0.395891	1.996158
H	1.102481	2.491667	-0.751292
H	0.642746	1.217330	-1.876248
H	-1.580444	2.082321	-1.533597
H	-1.133750	2.815598	0.016468
H	1.806467	1.895755	1.561867
H	2.162690	0.191136	1.899229
H	2.955134	1.009508	0.528538
O	1.947373	-0.809027	-1.560459
N	0.848264	-1.965993	0.076585
H	1.309663	-2.814187	-0.231339
H	0.582292	-1.907424	1.056959
H	-2.393540	0.853530	0.823369
O	-1.827103	-0.257849	-0.846084
O	-2.198169	-1.498812	-0.200420
H	-1.331825	-1.961091	-0.227511

DMPO-OOH C-O pos

N	-0.022942	-0.469890	-0.470223
C	-1.020166	0.610344	-0.511120
C	-0.184291	1.855701	-0.230195
C	0.986239	1.347178	0.639742
C	1.290606	-0.085084	0.138705
O	-1.959603	0.437230	0.536715
O	-2.856442	-0.637654	0.142262
C	1.640550	-1.061560	1.264754
C	2.362268	-0.113231	-0.965024
O	-0.376354	-1.692792	-0.626128
H	0.673544	1.309563	1.688383
H	1.864714	1.996193	0.575243
H	0.174874	2.263745	-1.181074
H	-0.783125	2.625030	0.262972
H	-1.547053	0.588261	-1.469448
H	0.859589	-1.064244	2.031787
H	1.740575	-2.077441	0.873433
H	2.587209	-0.768859	1.731633
H	3.347080	0.120460	-0.545338
H	2.405408	-1.108141	-1.419813
H	2.144894	0.614023	-1.755274

H -2.219160 -1.383707 0.055094
DEPMPO-OOH cis-3a

C 0.749880 -2.380738 0.294263
C 1.887384 -2.038115 -0.690090
C 2.540310 -0.769833 -0.127480
C 0.269239 -1.021456 0.848417
N 1.531214 -0.234937 0.798587
C -0.266985 -1.058056 2.280069
P -0.951377 -0.237513 -0.329816
O 1.764607 0.763299 1.555875
H 1.130204 -2.975789 1.133601
H -0.051101 -2.950997 -0.183470
H 1.472498 -1.798763 -1.672691
H 2.612535 -2.848196 -0.799149
H 0.491387 -1.491697 2.941218
H -0.490493 -0.048522 2.630917
O -2.327215 -0.924283 0.168210
C -3.515122 -0.869231 -0.666476
O -0.624932 -0.404845 -1.772529
C -4.408006 0.296317 -0.271816
H -5.324407 0.282455 -0.873851
H -4.686745 0.228836 0.784600
H -3.900153 1.251619 -0.432089
H -1.175254 -1.662394 2.328677
O 2.796607 0.089408 -1.222691
H 3.471303 -0.915528 0.430052
O -1.114746 1.287866 0.172544
C -0.325329 2.361842 -0.423414
C -0.223568 3.477136 0.598086
H -3.210418 -0.813100 -1.716233
H -4.019151 -1.826436 -0.505174
H 0.663195 1.988777 -0.700170
H -0.841570 2.683297 -1.333495
H 0.329496 4.321002 0.169980
H -1.217414 3.828678 0.894950
H 0.309854 3.123878 1.484672
O 3.677137 1.158003 -0.755988
H 4.369904 1.087362 -1.437932

CPCOMPO-OOH neg

C 0.050237 1.319763 -1.139449
C -1.322927 1.851892 -0.648680
C -1.815271 0.726655 0.256636
C 0.592246 0.451316 0.034290
N -0.574970 0.335782 0.925252
C 1.849351 0.955064 0.752655
C 1.039506 -0.955155 -0.426436
O -0.519180 -0.290384 2.033531
H 0.744441 2.126497 -1.390462
H -0.095775 0.704667 -2.030539
H -2.012300 2.040080 -1.474831
H -1.214050 2.771245 -0.064420
H 1.962109 2.042162 0.727172
H 1.797750 0.624231 1.794887

O 0.332801 -1.885700 -0.733528
C 2.971473 0.221451 0.009069
H 3.321847 0.767003 -0.874046
H 3.829467 -0.030746 0.634814
O 2.385809 -1.027366 -0.436291
H -2.559011 0.963815 1.021265
O -2.286478 -0.266611 -0.645295
O -2.456778 -1.512759 0.067769
H -1.586767 -1.922788 -0.138596

TAMPO-OOH pos

C 0.481923 -0.518117 -1.608595
C 1.755915 -1.163848 -1.004127
C 1.727533 -0.809435 0.482639
C -0.528050 -0.377094 -0.447038
N 0.281105 -0.725510 0.744246
C -1.827100 -1.209394 -0.508949
C -1.048754 1.068570 -0.221822
O -0.220431 -0.740974 1.917332
H 0.064682 -1.122301 -2.419180
H 0.721638 0.470282 -2.005330
H 2.668174 -0.799980 -1.478098
H 1.719666 -2.254367 -1.102405
H -2.116837 -1.338285 -1.556739
H -1.702574 -2.196903 -0.058899
O -0.371054 2.092888 -0.251551
C -2.886628 -0.362557 0.225450
H -3.880848 -0.456728 -0.222406
H -2.944865 -0.626638 1.286569
N -2.369255 0.993949 0.060026
H 2.139291 -1.568037 1.154336
O 2.431443 0.359055 0.862901
O 2.324080 1.371787 -0.172179
H 1.435665 1.770240 0.001907
H -2.848279 1.812841 0.412965

EMPO-OOH pos

C 0.467196 0.840051 1.650835
C 0.855937 -0.652703 1.713019
C 1.478595 -0.954860 0.351399
C 0.104457 1.119539 0.167180
N 0.877104 0.060232 -0.530760
C 0.510651 2.506273 -0.327101
O 1.227697 0.160614 -1.758152
H 1.325867 1.465256 1.915957
H -0.350805 1.091987 2.331687
H -0.027096 -1.282023 1.847820
H 1.563772 -0.870955 2.516189
H 1.575026 2.668655 -0.134526
H 0.331890 2.595152 -1.400787
H -0.075573 3.270289 0.188109
C -1.408204 0.905805 -0.061360
O -1.736385 -0.400612 -0.042706
C -3.143227 -0.704734 -0.230087

C	-3.290445	-2.213735	-0.213047
O	-2.207681	1.804145	-0.196595
H	-3.713845	-0.222364	0.569815
H	-3.466318	-0.268313	-1.179764
H	-4.341333	-2.483242	-0.363867
H	-2.699155	-2.673314	-1.011169
H	-2.964396	-2.631589	0.745079
O	2.878192	-0.754261	0.424087
H	1.279592	-1.951349	-0.052756
O	3.456219	-1.253588	-0.813473
H	3.028551	-0.653997	-1.466785

TFMPO-OOH neg

N	-0.597696	-0.476332	-0.274637
C	-1.584874	0.596418	-0.522794
C	-0.848219	1.859639	-0.086516
C	0.158040	1.379109	0.982053
C	0.555397	-0.057129	0.570857
O	-2.708150	0.406968	0.315453
O	-3.513157	-0.657994	-0.258826
C	0.755426	-1.023079	1.739719
C	1.812178	-0.045621	-0.319240
O	-0.926332	-1.706713	-0.409812
H	-0.326804	1.335141	1.961718
H	1.027838	2.034701	1.068836
H	-0.330105	2.288111	-0.947695
H	-1.552698	2.600255	0.298260
H	-1.903357	0.561176	-1.567965
H	-0.148868	-1.044064	2.353522
H	0.950140	-2.032521	1.372938
H	1.596791	-0.695935	2.356721
H	-2.889270	-1.415407	-0.184239
F	2.888314	0.372155	0.385602
F	2.089281	-1.265169	-0.808777
F	1.672808	0.793988	-1.371118

DiEtMPO-OOH pos (DEPO-OOH)

C	0.122636	0.397357	1.659349
C	0.496144	1.900859	1.764462
C	0.047288	2.487400	0.430506
C	0.068252	0.082002	0.129466
N	0.354207	1.390345	-0.486939
C	1.127646	-0.919811	-0.369323
O	0.902966	-1.835942	-1.124046
O	2.335934	-0.609551	0.126163
C	3.441188	-1.423964	-0.346243
C	4.707142	-0.886007	0.291129
H	-0.852969	0.207377	2.109968
H	0.853011	-0.237266	2.162954
H	1.578087	2.028389	1.861584
H	0.006462	2.392304	2.608559
H	3.468264	-1.365040	-1.438178
H	3.247094	-2.465159	-0.070432
H	4.653805	-0.944944	1.383078

H	4.874702	0.157538	0.006974
H	5.567078	-1.476322	-0.043106
C	-1.330363	-0.405462	-0.302894
O	-2.069540	0.191194	-1.058722
O	-1.635968	-1.553145	0.303936
C	-2.914886	-2.149600	-0.046024
H	-3.708798	-1.444088	0.217195
H	-2.936405	-2.296040	-1.129531
C	-3.026455	-3.456145	0.713956
H	-3.978758	-3.941026	0.473690
H	-2.213635	-4.135823	0.440530
H	-2.990135	-3.286910	1.794940
H	0.548311	3.389367	0.072309
O	-1.354423	2.686793	0.551623
O	-1.871273	3.063907	-0.746901
H	-2.039103	2.169795	-1.123554
O	0.568803	1.526201	-1.735141

CPPO-OOH neg

N	-0.608147	-0.409507	-0.511543
C	-1.695109	0.575392	-0.422012
C	-0.952920	1.873710	-0.114009
C	0.327930	1.422956	0.621437
C	0.708548	0.066869	-0.013212
O	-2.547717	0.255560	0.664444
O	-3.366964	-0.874060	0.254170
C	1.383471	-0.938134	0.937253
C	1.740400	0.176818	-1.163052
O	-0.856302	-1.641278	-0.766094
H	0.110038	1.283062	1.685521
H	1.133154	2.158952	0.538289
H	-0.712153	2.375470	-1.057464
H	-1.574801	2.548510	0.479048
H	-2.278177	0.562625	-1.347608
H	0.955175	-0.908458	1.944531
H	1.207060	-1.940609	0.533732
H	1.623455	-0.707800	-1.799893
H	1.581305	1.060480	-1.791342
H	-2.673418	-1.551357	0.081598
C	2.885390	-0.578707	0.896139
H	3.509074	-1.473949	0.982470
H	3.152441	0.070095	1.737540
C	3.111881	0.166577	-0.455652
H	3.875565	-0.315036	-1.074264
H	3.458617	1.189891	-0.272861

DiMAMPO-OOH pos

C	-0.531262	2.116776	0.094115
C	-1.558121	1.538298	-0.896611
C	-2.036565	0.260826	-0.214533
C	0.217598	0.883255	0.649370
N	-0.909869	-0.089473	0.678238
C	0.793426	1.121432	2.049862
C	1.351707	0.498328	-0.385380

O	-0.990474	-1.119277	1.438321	C	-2.024429	-0.923949	0.130128
H	-1.043110	2.615766	0.925539	C	0.291332	-0.054757	0.285998
H	0.154042	2.816825	-0.380309	N	-1.009482	0.007511	-0.405832
H	-1.067552	1.281151	-1.840164	C	1.049639	1.280548	0.433100
H	-2.386486	2.217742	-1.109095	O	-1.257815	0.705781	-1.454362
H	0.001071	1.455040	2.727193	H	0.663187	-1.089124	2.194423
H	1.248486	0.227048	2.477579	H	-0.478150	0.256695	2.291564
H	1.556275	1.905030	1.995051	H	-2.050790	-1.591042	2.193513
O	1.603373	1.306062	-1.278718	H	-0.994607	-2.530046	1.121174
N	2.052787	-0.669029	-0.266601	O	2.026089	1.309364	1.192104
C	1.913315	-1.706640	0.747746	N	0.603367	2.332404	-0.274250
H	-2.936264	0.375587	0.400727	H	-0.150718	2.153621	-0.933772
O	-2.253490	-0.760844	-1.157567	H	-2.289516	-1.640222	-0.651357
O	-2.960514	-1.840192	-0.482377	O	-3.170364	-0.197674	0.518674
H	1.006668	-1.583654	1.332985	O	-3.924589	0.114924	-0.685622
H	2.790530	-1.714179	1.410353	C	1.247940	3.634801	-0.229331
H	1.859637	-2.683835	0.251873	H	0.512582	4.415061	-0.007108
C	3.132682	-0.917837	-1.219270	H	2.004234	3.614076	0.555728
H	3.171065	-0.100803	-1.936222	H	1.730138	3.865966	-1.186383
H	4.092252	-0.990435	-0.690566	C	1.159503	-1.155214	-0.427491
H	2.955586	-1.864756	-1.743943	O	0.609172	-1.998532	-1.126688
H	-2.290475	-2.099630	0.188475	N	2.477694	-1.123105	-0.133341

MAMPO-OOH neg

C	1.142961	-1.440584	-0.949719
C	2.381449	-0.530697	-0.719507
C	1.841969	0.635360	0.101386
C	0.120136	-1.082827	0.163183
N	0.829554	-0.023986	0.925498
C	-0.229076	-2.252048	1.095332
C	-1.204181	-0.539317	-0.452413
O	0.372414	0.479856	2.010481
H	1.414317	-2.498404	-0.899592
H	0.690164	-1.265622	-1.926544
H	2.829811	-0.184968	-1.653941
H	3.154044	-1.043223	-0.137698
H	0.686301	-2.712809	1.480884
H	-0.823430	-1.904573	1.945164
H	-0.799527	-3.004071	0.542784
O	-1.672677	-1.031286	-1.467765
N	-1.800703	0.488588	0.233978
C	-3.167487	0.882855	-0.094033
H	2.534322	1.174054	0.751525
O	1.245849	1.512891	-0.850691
O	0.572026	2.579826	-0.141769
H	-1.463285	0.647601	1.180800
H	-3.903034	0.151959	0.265390
H	-3.263717	0.957310	-1.178299
H	-3.377742	1.854823	0.358640
H	-0.335706	2.208961	-0.112870

DiMAP-OOH neg

C	-0.155598	-0.588543	1.675596
C	-1.342792	-1.523625	1.364102

C	-2.024429	-0.923949	0.130128
C	0.291332	-0.054757	0.285998
N	-1.009482	0.007511	-0.405832
C	1.049639	1.280548	0.433100
O	-1.257815	0.705781	-1.454362
H	0.663187	-1.089124	2.194423
H	-0.478150	0.256695	2.291564
H	-2.050790	-1.591042	2.193513
H	-0.994607	-2.530046	1.121174
O	2.026089	1.309364	1.192104
N	0.603367	2.332404	-0.274250
H	-0.150718	2.153621	-0.933772
H	-2.289516	-1.640222	-0.651357
O	-3.170364	-0.197674	0.518674
O	-3.924589	0.114924	-0.685622
C	1.247940	3.634801	-0.229331
H	0.512582	4.415061	-0.007108
H	2.004234	3.614076	0.555728
H	1.730138	3.865966	-1.186383
C	1.159503	-1.155214	-0.427491
O	0.609172	-1.998532	-1.126688
N	2.477694	-1.123105	-0.133341
H	2.798332	-0.372062	0.472441
C	3.413995	-2.112738	-0.638615
H	4.211918	-1.632227	-1.215762
H	3.866873	-2.679787	0.183113
H	2.864192	-2.797034	-1.285899
H	-3.286217	0.698421	-1.151471

EMAPO-OOH neg

C	0.362983	-1.092622	1.560748
C	-0.234798	-2.403534	0.976814
C	-0.988761	-1.956824	-0.269676
C	0.370038	-0.065314	0.395897
N	-0.148364	-0.856465	-0.746153
C	-0.541313	1.162911	0.715529
O	-0.172068	-0.408648	-1.943153
H	1.369734	-1.257821	1.946416
H	-0.247251	-0.688888	2.369141
H	-0.897836	-2.909761	1.682200
H	0.554102	-3.100570	0.679314
O	-0.670891	1.563535	1.858954
N	-1.180043	1.709056	-0.366766
H	-0.788697	1.464704	-1.273193
H	-1.119666	-2.676300	-1.080461
O	-2.243155	-1.471681	0.196480
O	-2.954946	-0.888388	-0.920656
C	-1.811646	3.020088	-0.233879
H	-2.453619	3.195502	-1.100312
H	-2.415161	3.031361	0.674810
H	-1.065809	3.821224	-0.165157
C	1.758678	0.471715	0.007931
O	2.010040	1.640067	-0.178209
C	3.964310	-0.134665	-0.542232
H	4.538417	-1.059220	-0.599339

H 3.917456 0.353227 -1.518696
H 4.405806 0.552305 0.183818
O 2.644072 -0.529129 -0.119832
H -2.680008 0.049529 -0.823576

DEPMPO-O₂ trans mpw1K

C 1.212890 -1.691162 0.340218
C 2.173614 -1.366817 -0.810597
C 2.567262 0.062326 -0.526022
C 0.578962 -0.329725 0.676889
N 1.578794 0.605143 0.230195
C 0.235717 -0.125973 2.149733
P -0.967022 -0.106409 -0.367409
O 1.338064 1.929603 0.329070
H 1.766785 -2.036441 1.219642
H 0.476182 -2.456470 0.083052
H 1.647017 -1.400452 -1.769152
H 3.041873 -2.028783 -0.859779
H 1.127533 -0.347246 2.744577
H -0.030283 0.920333 2.312042
O -1.948439 -1.240033 0.289135
C -3.207449 -1.485607 -0.335751
O -0.781628 -0.255409 -1.840044
C -3.857370 -2.665535 0.354505
H -4.830132 -2.880165 -0.099360
H -3.230107 -3.556430 0.267241
H -4.008836 -2.456086 1.416618
H -0.586917 -0.771461 2.467919
O -1.806785 1.213549 0.055234
C -1.470535 2.483888 -0.549179
C -2.224827 3.556412 0.202112
H -3.832808 -0.589682 -0.247947
H -3.049849 -1.688782 -1.400675
H -0.380746 2.611379 -0.464232
H -1.767411 2.447656 -1.602708
H -2.016125 4.533559 -0.245254
H -3.306401 3.386785 0.173427
H -1.904390 3.585171 1.246585
O 3.946717 -0.005714 0.362061
H 2.927156 0.677768 -1.352626
O 4.922278 -0.544165 -0.320587

DEPMPO-O₂ trans mpw1K neg

C 1.418611 -1.380108 0.034780
C 2.386982 -0.871654 -1.047238
C 2.378200 0.587807 -0.816647
C 0.595214 -0.149623 0.468467
N 1.380787 0.984906 -0.076522
C 0.441767 0.007021 1.975423
P -1.051096 -0.142525 -0.378291
O 1.035442 2.198552 0.241536
H 1.997303 -1.721506 0.897295
H 0.792290 -2.209256 -0.300830
H 2.034130 -1.109426 -2.059066

H 3.405105 -1.270508 -0.897621
H 1.438764 0.006137 2.423896
H -0.044333 0.954254 2.211141
O -1.736421 -1.428788 0.338537
C -2.999954 -1.886185 -0.151154
O -1.025397 -0.196371 -1.864801
C -3.282237 -3.239510 0.462728
H -4.250351 -3.614333 0.116547
H -2.510376 -3.959200 0.179663
H -3.306273 -3.172466 1.553301
H -0.141379 -0.820117 2.386236
O -1.989059 1.030560 0.219505
C -1.976034 2.338164 -0.396330
C -2.927633 3.215464 0.383622
H -3.771955 -1.160021 0.127336
H -2.961974 -1.946944 -1.243728
H -0.948773 2.716491 -0.360367
H -2.292030 2.230372 -1.438501
H -2.955241 4.214471 -0.062213
H -3.942473 2.806200 0.379268
H -2.596969 3.313379 1.420568
O 4.538085 0.215588 0.479946
H 3.007503 1.328924 -1.283650
O 5.044659 -0.953438 0.170131

DEPMPO-O₂ trans mpw1K pos

C 1.342303 -1.581489 -0.036882
C 2.308315 -1.075635 -1.112257
C 2.767960 0.256881 -0.542720
C 0.640208 -0.313845 0.499338
N 1.531243 0.764171 0.039846
C 0.471348 -0.277569 2.016940
P -0.986694 -0.112324 -0.357562
O 1.381613 1.967627 0.443619
H 1.912148 -2.023005 0.784835
H 0.634620 -2.328831 -0.404714
H 1.802399 -0.939995 -2.072325
H 3.197748 -1.702150 -1.213659
H 1.463267 -0.382199 2.463782
H 0.042714 0.674744 2.334136
O -1.846346 -1.296386 0.345439
C -3.150157 -1.588530 -0.165028
O -0.979026 -0.149864 -1.845437
C -3.591746 -2.919907 0.401145
H -4.594616 -3.167402 0.039869
H -2.906582 -3.714021 0.095060
H -3.614865 -2.887888 1.493344
H -0.172510 -1.093726 2.352272
O -1.752463 1.183426 0.243865
C -1.614523 2.463262 -0.403743
C -2.665353 3.385500 0.171424
H -3.834986 -0.787668 0.136054
H -3.111043 -1.616240 -1.258753
H -0.603872 2.833045 -0.212128
H -1.746734 2.326580 -1.481097

H -2.583751 4.373021 -0.292930
 H -3.672497 2.999455 -0.010422
 H -2.528523 3.501620 1.249567
 O 3.674337 0.089428 0.509512
 H 3.151238 0.965855 -1.290529
 O 4.796563 -0.642673 -0.021640

DEPMPO-O₂ trans B3LYP

C 1.263365 -1.668721 0.069698
 C 2.249696 -1.241908 -1.037108
 C 2.634674 0.153312 -0.595791
 C 0.596975 -0.344852 0.521857
 N 1.530601 0.670330 0.038309
 C 0.376351 -0.216637 2.033946
 P -1.016344 -0.127044 -0.408565
 O 1.409747 1.952273 0.419292
 H 1.818932 -2.077068 0.920915
 H 0.543422 -2.426064 -0.257608
 H 1.756859 -1.211413 -2.015242
 H 3.137814 -1.878633 -1.090867
 H 1.330340 -0.421095 2.533617
 H 0.087139 0.811970 2.261263
 O -1.974683 -1.241716 0.327182
 C -3.294079 -1.453987 -0.194776
 O -0.941061 -0.273186 -1.892926
 C -3.905390 -2.640695 0.532463
 H -4.921292 -2.832676 0.165409
 H -3.302231 -3.541034 0.373878
 H -3.955383 -2.448629 1.609656
 H -0.387028 -0.911872 2.397584
 O -1.775753 1.225467 0.086578
 C -1.400467 2.501141 -0.507366
 C -2.130375 3.585224 0.264064
 H -3.893768 -0.548240 -0.038274
 H -3.233137 -1.639030 -1.273924
 H -0.308839 2.606447 -0.414440
 H -1.700676 2.489460 -1.561922
 H -1.908380 4.567398 -0.171790
 H -3.216973 3.434004 0.241853
 H -1.802386 3.592724 1.308839
 O 3.834646 -0.027607 0.507356
 H 3.101860 0.820750 -1.322931
 O 4.827128 -0.786596 0.011564

DEPMPO-O₂ trans B3LYP neg

C 1.414133 -1.421244 0.024726
 C 2.376267 -0.937617 -1.086085
 C 2.421669 0.524889 -0.834190
 C 0.601519 -0.169201 0.445213
 N 1.408278 0.952938 -0.112116
 C 0.454345 0.015436 1.956835
 P -1.051542 -0.145939 -0.409118
 O 1.089747 2.189477 0.201001
 H 2.012340 -1.742757 0.883263

H 0.778781 -2.258344 -0.278855
 H 1.989550 -1.163133 -2.091085
 H 3.379913 -1.376565 -0.950840
 H 1.452298 -0.032819 2.405948
 H 0.027087 0.997773 2.167518
 O -1.772621 -1.413846 0.333726
 C -3.082840 -1.808183 -0.102943
 O -1.024391 -0.220492 -1.897593
 C -3.396719 -3.162717 0.510345
 H -4.398860 -3.493684 0.211323
 H -2.669349 -3.911525 0.179939
 H -3.360162 -3.109180 1.603667
 H -0.176888 -0.767052 2.389000
 O -1.970856 1.057937 0.183503
 C -1.890209 2.375576 -0.428707
 C -2.655784 3.333785 0.465041
 H -3.808940 -1.051325 0.219512
 H -3.101906 -1.856276 -1.198060
 H -0.831833 2.652163 -0.499895
 H -2.335807 2.316834 -1.428504
 H -2.655597 4.337724 0.022907
 H -3.696474 3.013319 0.596578
 H -2.183145 3.392985 1.450803
 O 4.392753 0.148058 0.524611
 H 3.033659 1.256924 -1.339647
 O 4.911148 -1.034994 0.264328

DEPMPO-O₂ trans B3LYP pos

C 1.304717 -1.634243 -0.080991
 C 2.324697 -1.151968 -1.130756
 C 2.752844 0.197797 -0.566447
 C 0.624376 -0.339336 0.443416
 N 1.515805 0.729084 -0.057162
 C 0.479424 -0.274860 1.970038
 P -1.017237 -0.122664 -0.405939
 O 1.449999 1.941176 0.449674
 H 1.836089 -2.099496 0.755014
 H 0.589957 -2.364218 -0.474798
 H 1.860640 -1.038770 -2.116098
 H 3.210610 -1.789779 -1.184898
 H 1.476411 -0.413430 2.400735
 H 0.108552 0.708863 2.266512
 O -1.923813 -1.258734 0.351285
 C -3.260955 -1.490684 -0.116237
 O -1.024223 -0.221250 -1.894639
 C -3.769842 -2.772617 0.522546
 H -4.798244 -2.977505 0.200359
 H -3.139411 -3.620867 0.235895
 H -3.757487 -2.691146 1.614732
 H -0.198011 -1.051004 2.340193
 O -1.747168 1.216982 0.168528
 C -1.455810 2.503267 -0.438807
 C -2.320357 3.538059 0.258949
 H -3.890662 -0.636028 0.162800
 H -3.255786 -1.568381 -1.209725

H	-0.388330	2.708118	-0.301554
H	-1.688257	2.445126	-1.508292
H	-2.143972	4.528972	-0.177318
H	-3.385953	3.299307	0.157965
H	-2.076531	3.584355	1.325619
O	3.642714	0.025916	0.550913
H	3.207892	0.882389	-1.296576
O	4.728222	-0.781917	0.140286

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