

## **Supplementary Information**

### **Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide (DMPO). 3. Effect of Mildly Acidic pH on the Thermodynamics and Kinetics of Adduct Formation**

**Randy A. Burgett, Xiaofeng Bao and Frederick A. Villamena\***

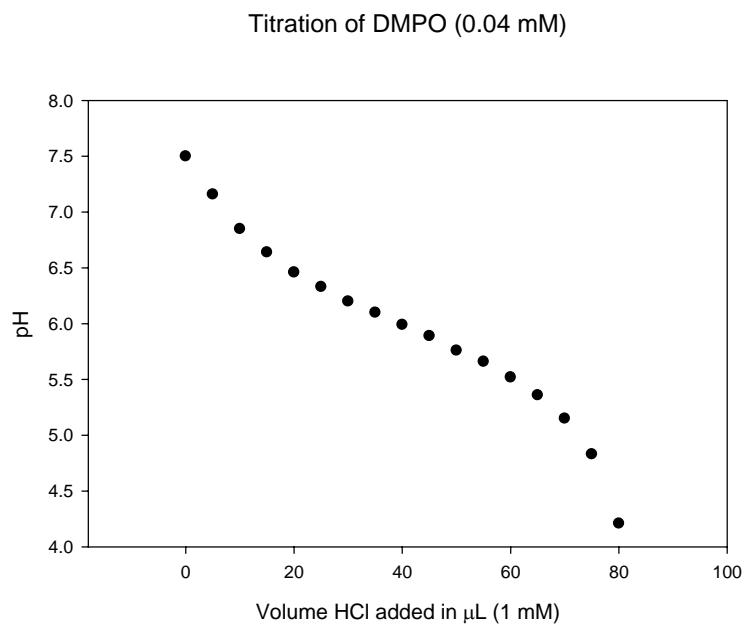
*Department of Pharmacology and Davis Heart and Lung Research Institute,  
The Ohio State University, Columbus, OH, 43210*

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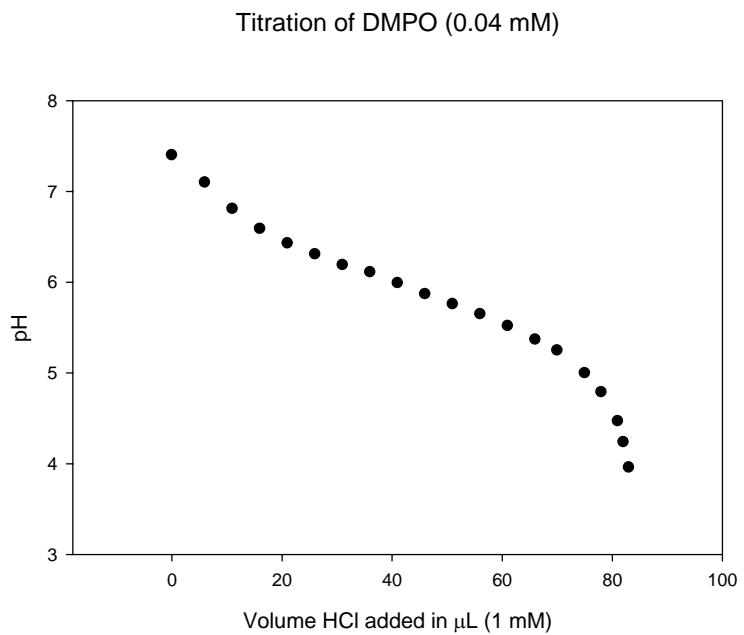
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\* Correspondence to: Frederick.Villamena@osumc.edu; Fax: 614-688-0999

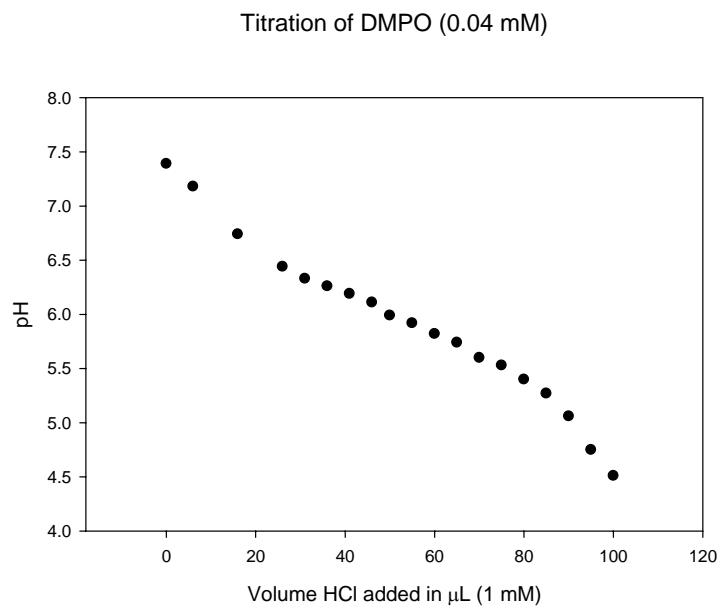
**Table S1.** Potentiometric Titration Trial 1

Titrant ( $\mu\text{L}$ )	pH	Stoichiometric Concentrations		$[\text{DMPO-H}^+]/[\text{DMPO}]$	$\log ([\text{DMPO-}\text{H}^+]/[\text{DMPO}])$	$\text{pK}_a$
		$[\text{DMPO-H}^+]$ (mM)	$[\text{DMPO}]$ (mM)			
0.0	7.50	0.000	0.040			
5.0	7.16	0.003	0.038	0.067	-1.176	5.984
10.0	6.85	0.005	0.035	0.143	-0.845	6.005
15.0	6.64	0.008	0.033	0.231	-0.637	6.003
20.0	6.46	0.010	0.030	0.333	-0.477	5.983
25.0	6.33	0.013	0.028	0.455	-0.342	5.988
30.0	6.20	0.015	0.025	0.600	-0.222	5.978
35.0	6.10	0.018	0.023	0.778	-0.109	5.991
40.0	5.99	0.020	0.020	1.000	0.000	5.990
45.0	5.89	0.023	0.018	1.286	0.109	5.999
50.0	5.76	0.025	0.015	1.667	0.222	5.982
55.0	5.66	0.028	0.013	2.200	0.342	6.002
60.0	5.52	0.030	0.010	3.000	0.477	5.997
65.0	5.36	0.033	0.008	4.333	0.637	5.997
70.0	5.15	0.035	0.005	7.000	0.845	5.995
75.0	4.83	0.038	0.003	15.000	1.176	6.006
80.0	4.21	0.040	0.000		Average	<b><math>5.993 \pm 0.009</math></b>

**Table S2.** Potentiometric Titration Trial 2

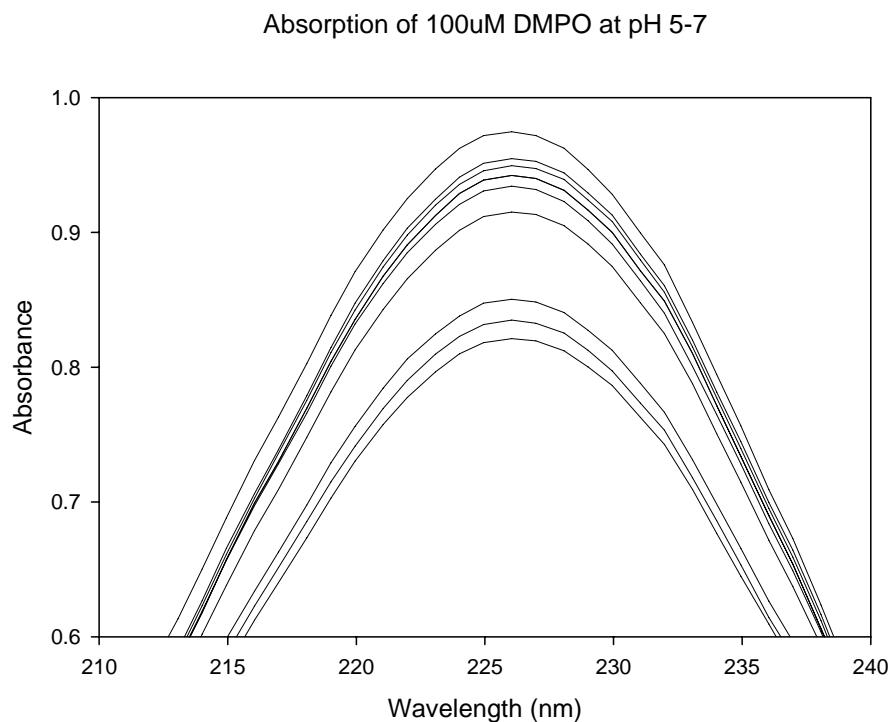
Titrant (uL)	pH	Stoichiometric Concentrations			$\log \left( \frac{[\text{DMPO-H}^+]}{[\text{DMPO}]} \right)$	$pK_a$
		[DMPO-H <sup>+</sup> ] (mM)	[DMPO] (mM)	$[\text{DMPO-H}^+]/[\text{DMPO}]$		
0.0	7.40	0.000	0.040			
6.0	7.10	0.003	0.037	0.081	-1.093	6.007
11.0	6.81	0.006	0.035	0.159	-0.797	6.013
16.0	6.59	0.008	0.032	0.250	-0.602	5.988
21.0	6.43	0.010	0.030	0.351	-0.454	5.976
26.0	6.31	0.013	0.027	0.471	-0.327	5.983
31.0	6.19	0.015	0.025	0.619	-0.208	5.982
36.0	6.11	0.018	0.022	0.794	-0.100	6.010
41.0	5.99	0.020	0.020	1.010	0.004	5.994
46.0	5.87	0.023	0.018	1.286	0.109	5.979
51.0	5.76	0.025	0.015	1.649	0.217	5.977
56.0	5.65	0.027	0.013	2.125	0.327	5.977
61.0	5.52	0.030	0.010	3.000	0.477	5.997
66.0	5.37	0.032	0.008	3.938	0.595	5.965
70.0	5.25	0.034	0.006	5.452	0.737	5.987
75.0	5.00	0.036	0.004	9.256	0.966	5.966
78.0	4.79	0.038	0.002	15.620	1.190	5.980
81.0	4.47	0.039	0.001	35.364	1.549	6.019
82.0	4.24	0.039	0.001	56.143	1.749	5.989
83.0	3.96	0.040	0.000		Average	<b>5.988 ± 0.015</b>

**Table S3.** Potentiometric Titration Trial 3



Titrant (uL)	Stoichiometric Concentrations				$\log ([\text{DMPO}-\text{H}^+]/[\text{DMPO}])$	$\text{pK}_a$
	pH	[DMPO-H <sup>+</sup> ] (mM)	[DMPO] (mM)	$[\text{DMPO}-\text{H}^+]/[\text{DMPO}]$		
0.0000	7.3900	0.0000	0.0400			
6.0000	7.1800	0.0024	0.0376	0.0638	-1.1950	5.9850
16.0000	6.7400	0.0064	0.0336	0.1905	-0.7202	6.0198
26.0000	6.4400	0.0104	0.0296	0.3514	-0.4543	5.9857
31.0000	6.3300	0.0124	0.0276	0.4493	-0.3475	5.9825
36.0000	6.2600	0.0144	0.0256	0.5625	-0.2499	6.0101
41.0000	6.1900	0.0164	0.0236	0.6949	-0.1581	6.0319
46.0000	6.1100	0.0184	0.0216	0.8519	-0.0696	6.0404
50.0000	5.9900	0.0200	0.0200	1.0000	0.0000	5.9900
55.0000	5.9200	0.0220	0.0180	1.2222	0.0872	6.0072
60.0000	5.8200	0.0240	0.0160	1.5000	0.1761	5.9961
65.0000	5.7400	0.0260	0.0140	1.8571	0.2688	6.0088
70.0000	5.6600	0.0280	0.0120	2.3333	0.3680	5.9680
75.0000	5.5300	0.0300	0.0100	3.0000	0.4771	6.0071
80.0000	5.4000	0.0320	0.0080	4.0000	0.6021	6.0021
85.0000	5.2700	0.0340	0.0060	5.6667	0.7533	6.0233
90.0000	5.0600	0.0360	0.0040	9.0000	0.9542	6.0142
95.0000	4.7500	0.0380	0.0020	19.0000	1.2788	6.0288
100.0000	4.5100	0.0400	0.0000			
					Average	<b><math>6.006 \pm 0.020</math></b>

**Table S4.** Spectrophotometric Titration Trial 1



$A$  = absorbances at pH 5.1-6.9;  $A_I$  = absorption of  $\text{DMPO-H}^+$ ;  $A_M$  = absorption of DMPO

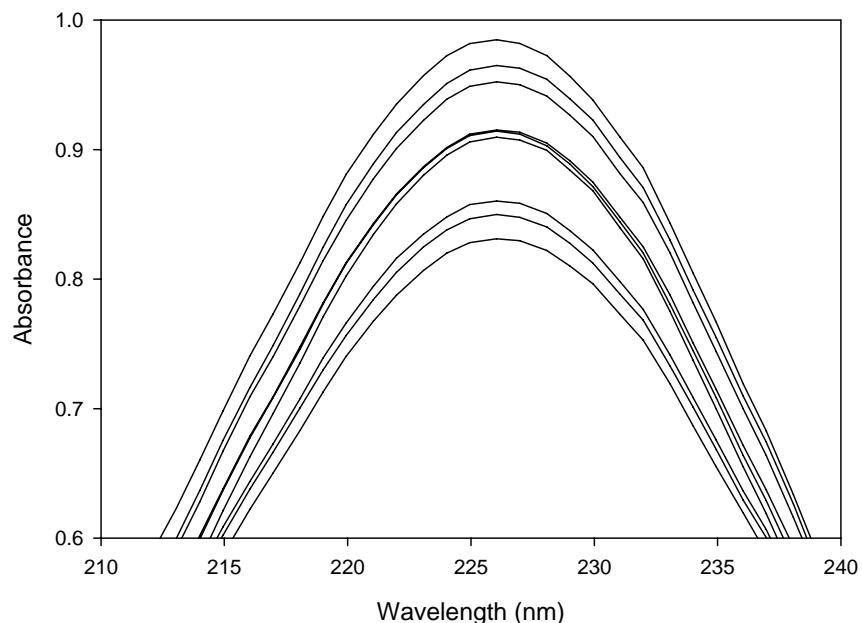
pH	A	$A_I - A$	$A - A_m$	$\log [A - A_m]/[ A_I - A]$	$pK_a$
6.8800	0.8300	0.1500	0.0200	-0.8751	6.0049
6.5000	0.8500	0.1300	0.0400	-0.5119	5.9881
5.8700	0.9100	0.0700	0.1000	0.1549	6.0249
5.6000	0.9300	0.0500	0.1200	0.3802	5.9802
5.4600	0.9400	0.0400	0.1300	0.5119	5.9719
5.3300	0.9500	0.0300	0.1400	0.6690	5.9990
5.1300	0.9600	0.0200	0.1500	0.8751	6.0051

Average  
5.9963

Standard Deviation  
0.0178

**Table S5.** Spectrophotometric Titration Trial 2

Absorption of 100uM DMPO at pH 5-7



$A$  = absorbances at pH 5.1-6.9;  $A_I$  = absorption of  $\text{DMPO-H}^+$ ;  $A_M$  = absorption of DMPO

pH	A	$A_I - A$	$A - A_m$	$\log [A - A_m]/[ A_I - A ]$	$pK_a$
6.8200	0.8500	0.1300	0.0200	-0.8129	6.0071
6.6300	0.8600	0.1200	0.0300	-0.6021	6.0279
5.9800	0.9100	0.0700	0.0800	0.0580	6.0380
5.8600	0.9150	0.0650	0.0850	0.1165	5.9765
5.8100	0.9170	0.0630	0.0870	0.1402	5.9502
5.4200	0.9500	0.0300	0.1200	0.6021	6.0221
5.0400	0.9650	0.0150	0.1350	0.9542	5.9942

Average  
6.0023

Standard Deviation  
0.0311

**Table S6.**  $^1\text{H}$ -NMR  $\text{p}K_{\text{a}}$  Determination
 $\delta_{\text{A}}$  = chemical shift of DMPO- $\text{H}^+$ ;  $\delta_{\text{B}}$  = chemical shift of DMPO

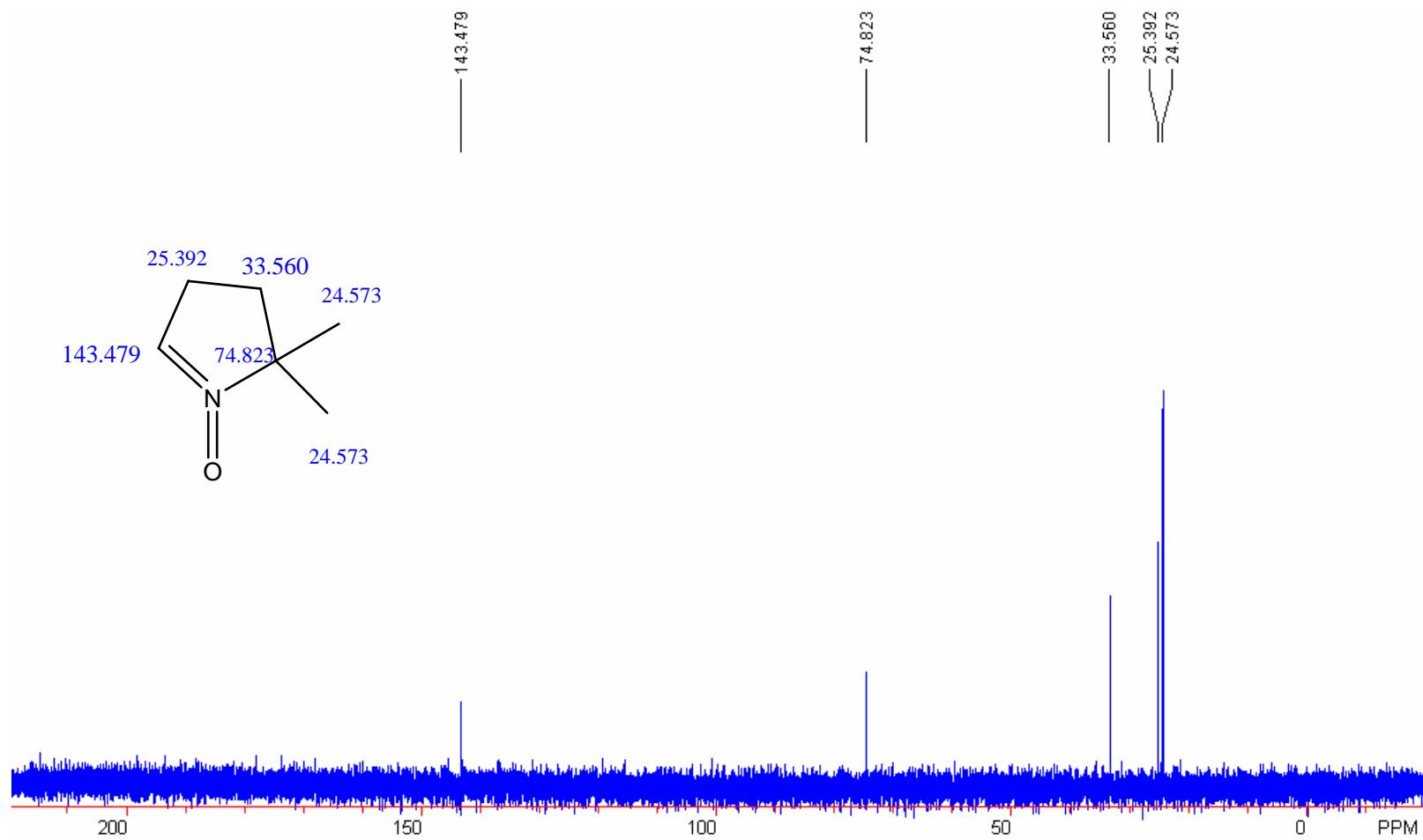
pH	$\delta$ (ppm)	$\delta_{\text{A}} - \delta$	$\delta - \delta_{\text{B}}$	$\log(\delta - \delta_{\text{B}}/\delta_{\text{A}} - \delta)$	$\text{p}K_{\text{a}}$
7.00	7.1190				
6.85	7.1300	0.0410	0.0110	-0.5714	6.2786
6.00	7.1450	0.0260	0.0260	0.0000	6.0000
5.10	7.1710				
<b>Average = 6.14 ± 0.20</b>					

**Table S7.**  $^{13}\text{C}$ -NMR  $\text{p}K_{\text{a}}$  Determination
 $\delta_{\text{A}}$  = chemical shift of DMPO- $\text{H}^+$ ;  $\delta_{\text{B}}$  = chemical shift of DMPO

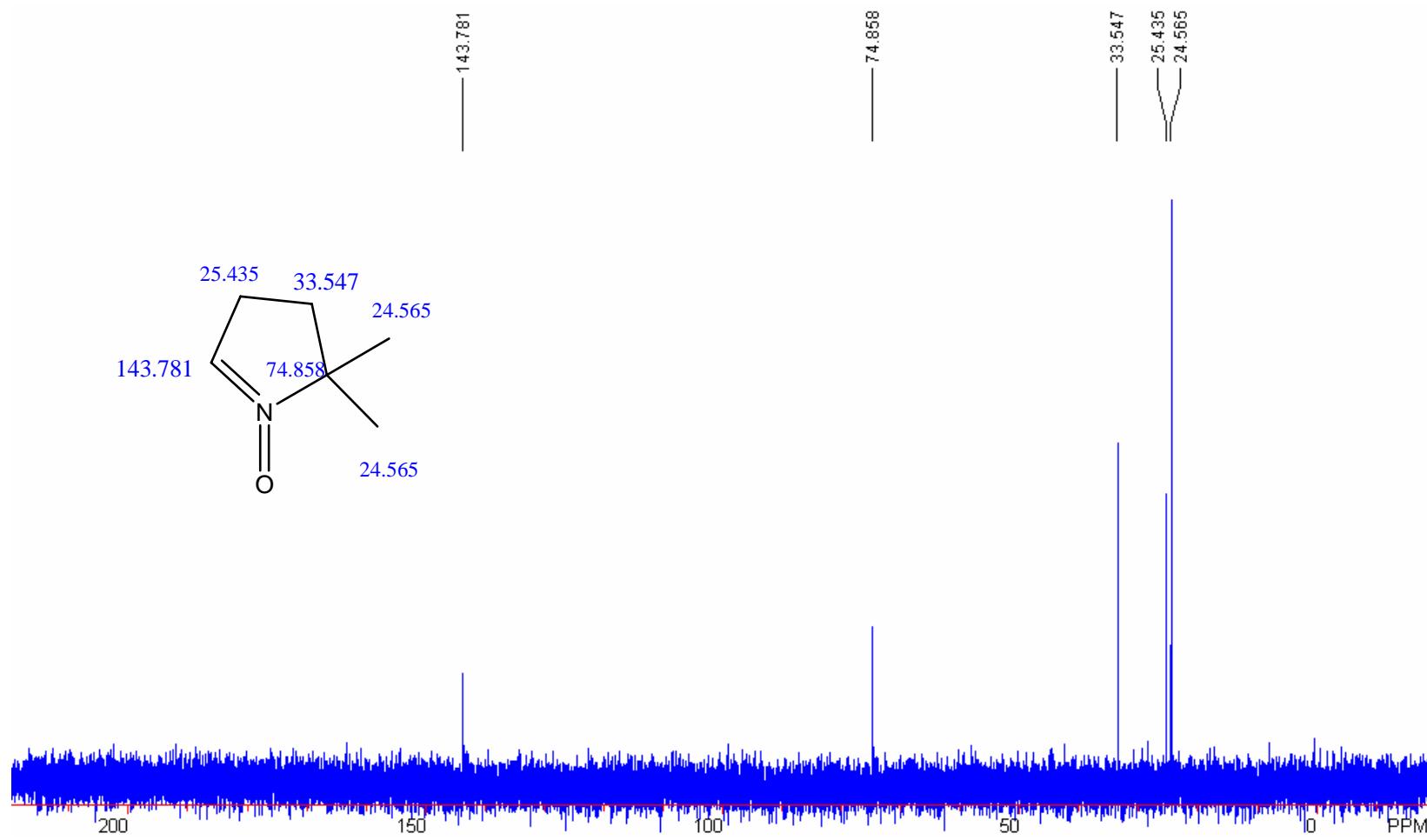
pH	$\delta$ (ppm)	$\delta_{\text{A}} - \delta$	$\delta - \delta_{\text{B}}$	$\log(\delta - \delta_{\text{B}}/\delta_{\text{A}} - \delta)$	$\text{p}K_{\text{a}}$
7.10	143.479				
6.50	143.781	0.776	0.302	-0.4099	6.0902
6.00	144.112	0.445	0.633	0.1530	6.1530
4.90	144.557				
<b>Average = 6.12 ± 0.04</b>					

pH	$\delta$ (ppm)	$\delta_{\text{A}} - \delta$	$\delta - \delta_{\text{B}}$	$\log(\delta - \delta_{\text{B}}/\delta_{\text{A}} - \delta)$	$\text{p}K_{\text{a}}$
7.10	74.823				
6.50	74.858	0.100	0.035	-0.4559	6.044
6.00	74.901	0.057	0.078	0.1362	6.136
4.90	74.958				
<b>Average = 6.09 ± 0.07</b>					

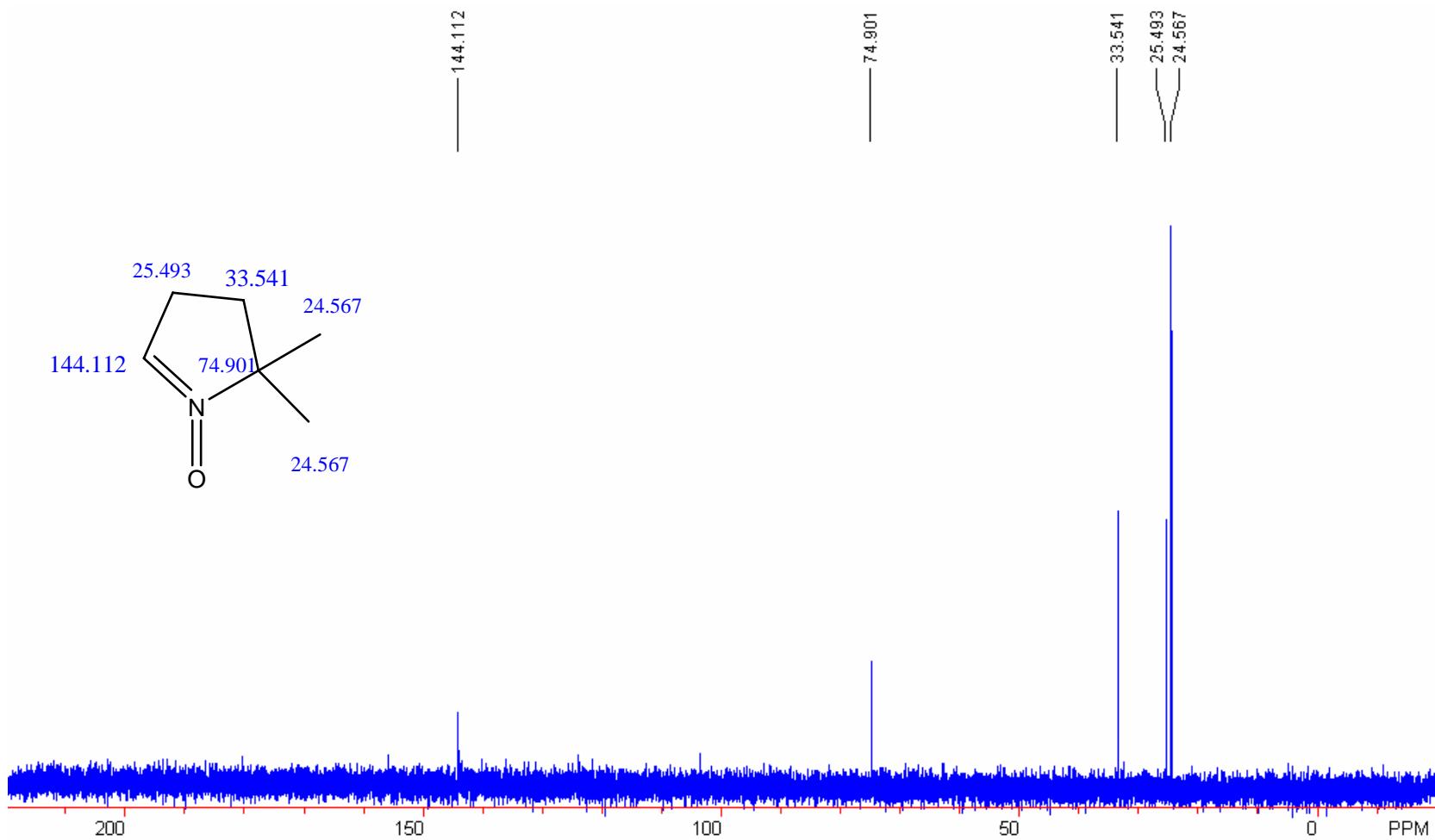
**Figure S1.**  $^{13}\text{C}$ -NMR at pH 7.1



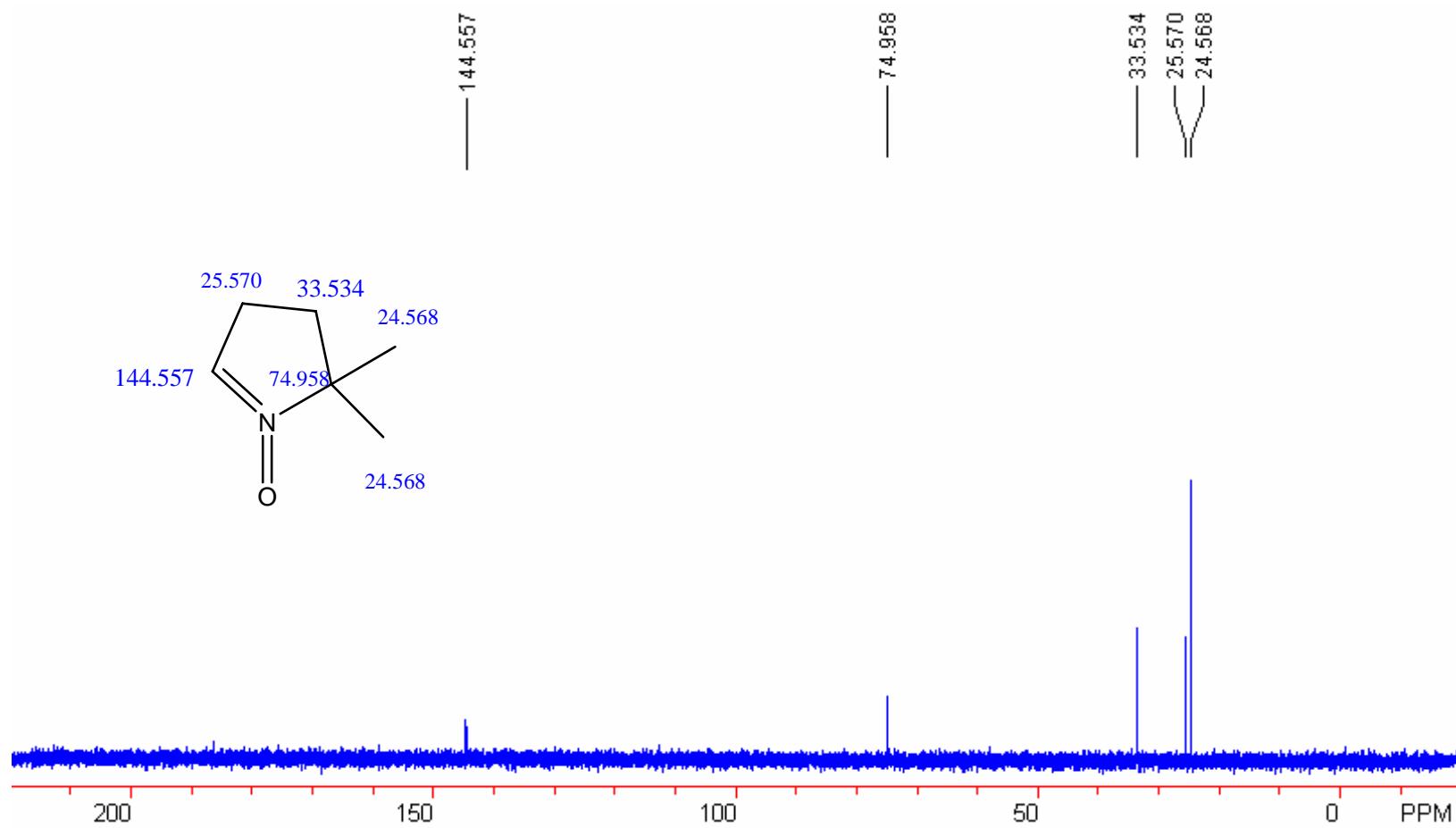
**Figure S2.**  $^{13}\text{C}$ -NMR at pH 6.50



**Figure S3.**  $^{13}\text{C}$ -NMR at pH 6.0



**Figure S4.**  $^{13}\text{C}$ -NMR at pH 4.9



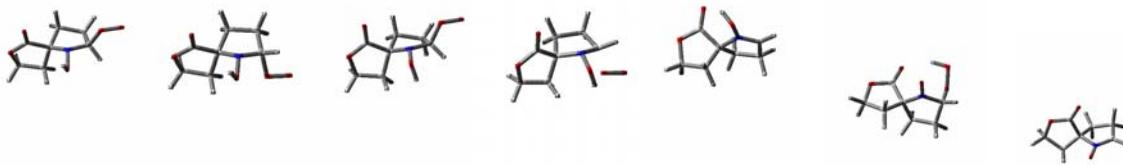
**Table S8.** Thermodynamic data for nitrones, nitrone-H<sup>+</sup>, nitrone-H<sup>+</sup>-O<sub>2</sub>, and nitrone-O<sub>2</sub>H at the PCM/B3LYP/6-31+G\*\*//B3LYP/6-31G\* level at 298 K.

pcm/b3lyp/6-31+g\*\*//b3lyp/6-31g\*

ZPE scaling factor = 0.980600      hartree to kcal/mol = 627.5095



Compound file	AMPO-H-OO cis AMPO-H-O2-cis.log	AMPO-H-OO trans AMPO-H-O2-trans.log	AMPO-H-OO cis AMPO-H-O2-cis-b.log	AMPO-H-OO trans AMPO-H-O2-trans-b.log	AMPO-H	AMPO-H-b	AMPO-OOH disamo-ho2TS_dneg.log	AMPO conh2.log
E 6-31+g** tight PCM	-645.547627	-645.545855	-645.545686	-645.543341	-495.038652	-495.05308	-645.5678110	-494.613836
E 6-31g*	-645.478373	-645.477421	-645.4771384	-645.4807158	-494.9220087	-494.9367606	-645.5074985	-494.5653155
ZPE (raw)	0.184119	0.184070	0.183845	0.184079	0.178374	0.178069	0.1856020	0.166017
Therm Corr to H (raw)	0.197554	0.197602	0.197246	0.197496	0.18903	0.188696	0.1983080	0.176458
Therm Corr to G (raw)	0.144364	0.144250	0.144202	0.143955	0.14376	0.14368	0.1479320	0.13143
H (raw)								-494.388857
G (raw)								-494.433885
ZPE (scaled)	0.180547	0.180499	0.180278	0.180508	0.174914	0.174614	0.1820013	0.162796
Electronic State	2-A	2-A	2-A	2-A	1-A	1-A	2-A	
s2 6-31g*	0.754200	0.754200	0.7542	0.7542	0	0	0.7544000	0.000000
Symmetry	C1	C1	C1	C1	C1	C1	C1	C01
N Imag	0.000000	0.000000	0	0	0	#NAME?	0.000000	0.000000
Rotational Con. (GHz)	1.656020	1.740637	1.616523	1.7475291	1.8466015	1.908557	1.1936742	1.755748
Rotational Con. (GHz)	0.638844	0.682114	0.6386132	0.6746832	1.2687394	1.2900304	0.9454383	1.375520
Rotational Con. (GHz)	0.575352	0.596841	0.6134735	0.5961197	1.0675034	1.0063902	0.8284154	1.109713
H298								
6-31+g** tight PCM	-645.353645	-645.351824	-645.352007	-645.349416	-494.853082	-494.867839	-645.3731037	-494.440599
6-31g* tight	-645.284390	-645.283390	-645.283459	-645.286791	-494.736439	-494.751519	-645.3127912	-494.392078
G298	-7.411119	-6.370112	-6.291444	-4.977778				
6-31+g** tight PCM	-645.406835	-645.405176	-645.405051	-645.402957	-494.898352	-494.912855	-645.4234797	-494.485627
6-31g* tight	-645.337580	-645.336742	-645.336503	-645.340332	-494.781709	-494.796535	-645.3631672	-494.437106



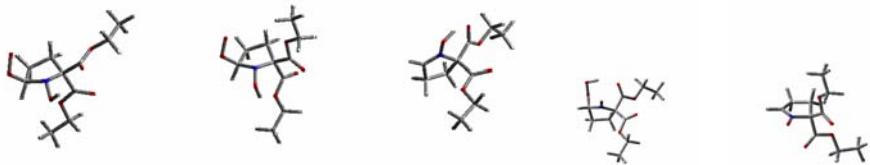
Compound file	CPCOMPO-H-OO cis	CPCOMPO-H-OO trans	CPCOMPO-H-OO cis	CPCOMPO-H-OO trans	CPCOMPO-H-CPCOMPO-H2-cis.log	CPCOMPO-H-CPCOMPO-H2-trans.log	CPCOMPO-OOH	CPCOMPO
<b>E 6-31+g** tight PCM</b>	-703.506651	-703.504939	-703.501238	-703.498152	-552.995678	-703.5259570	-703.5259570	-552.567088
<b>E 6-31g*</b>	-703.443544	-703.444454	-703.4325735	-703.4421866	-552.881420	-703.4702272	-703.4702272	-552.5210662
<b>ZPE (raw)</b>	0.179827	0.180005	0.179304	0.179814	0.173702	0.1807830	0.1807830	0.161224
<b>Therm Corr to H (raw)</b>	0.192591	0.192790	0.192118	0.192446	0.183915	0.1930520	0.1930520	0.171253
<b>Therm Corr to G (raw)</b>	0.140578	0.140778	0.13996	0.140876	0.139329	0.1431440	0.1431440	0.126635
<b>H (raw)</b>								-552.349813
<b>G (raw)</b>								-552.394431
<b>ZPE (scaled)</b>	0.176338	0.176513	0.175826	0.176326	0.170332	0.1772758	0.1772758	0.158096
<b>Electronic State</b>	2-A	2-A	2-A	2-A	1-A	2-A	2-A	2-A
<b>s2 6-31g*</b>	0.754200	0.754200	0.7542	0.7545	0.000000	0.7543000	0.7543000	0.000000
<b>Symmetry</b>	C1	C1	C1	C1	C1	C1	C1	C01
<b>N Imag</b>	0.000000	0.000000	0	0.000000	#NAME?	0.0000000	0.0000000	0.000000
<b>Rotational Con. (GHz)</b>	1.631296	1.477936	1.6090199	1.365421	1.754736	1.3468049	1.3468049	1.777462
<b>Rotational Con. (GHz)</b>	0.537063	0.593456	0.5349191	0.6456491	1.067075	0.7261906	0.7261906	1.050776
<b>Rotational Con. (GHz)</b>	0.510218	0.569607	0.5157277	0.613747	0.891901	0.6403753	0.6403753	0.972269
<b>H298</b>								
<b>6-31+g** tight PCM</b>	-703.317549	-703.315641	-703.312598	-703.309194	-552.815133	-703.3364122	-703.3364122	-552.398963
<b>6-31g* tight</b>	-703.254441	-703.255156	-703.243934	-703.253229	-552.700875	-703.2806824	-703.2806824	-552.352941
<b>G298</b>	-17.364961	-16.167329	-14.349686	-11.844601				
<b>6-31+g** tight PCM</b>	-703.369562	-703.367653	-703.364756	-703.360764	-552.859719	-703.3863202	-703.3863202	-552.443581
<b>6-31g* tight</b>	-703.306454	-703.307168	-703.296092	-703.304799	-552.745461	-703.3305904	-703.3305904	-552.397559



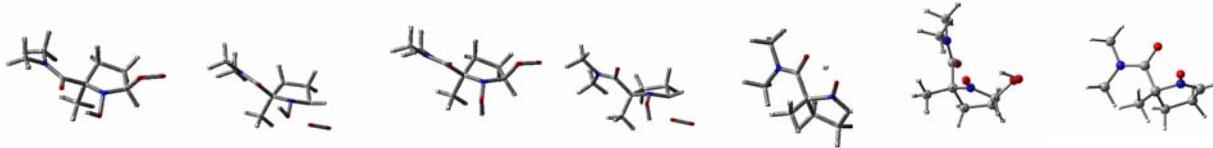
<b>Compound</b>	<b>CPPO-H-OO</b>	<b>CPPO-H-OO-b</b> CPPO-H-O2- b.log	<b>CPPO-H</b>	<b>CPPO-OOH</b> CPPO2H- b3lyp_neg_d.log	<b>CPPO</b>
<b>file</b>	CPPO-H-O2.log		CPPO-H.log	b3lyp_neg_d.log	CPPO.log
<b>E 6-31+g** tight PCM</b>	-593.561802	-593.55654	-443.067853	-593.5861730	-442.628213
<b>E 6-31g*</b>	-593.510184	-593.5125387	-442.9600159	-593.5394310	-442.5911999
<b>ZPE (raw)</b>	0.222356	0.222261	0.215931	0.2231210	0.203852
<b>Therm Corr to H (raw)</b>	0.235058	0.234804	0.226354	0.2354700	0.213742
<b>Therm Corr to G (raw)</b>	0.182796	0.182733	0.181207	0.1845330	0.169114
<b>H (raw)</b>					-442.377458
<b>G (raw)</b>					-442.422085
<b>ZPE (scaled)</b>	0.218042	0.217949	0.211742	0.2187925	0.199897
<b>Electronic State</b>	2-A	2-A	1-A	2-A	
<b>s2 6-31g*</b>	0.754300	0.7546	0	0.7539000	
<b>Symmetry</b>	C1	C1	C1	-	C01
<b>N Imag</b>	0.000000	0	#NAME?	0.0000000	0.000000
<b>Rotational Con. (GHz)</b>	1.676574	1.578961	2.1775307	1.9088034	2.260288
<b>Rotational Con. (GHz)</b>	0.661172	0.7291421	1.1318322	0.6379774	1.154036
<b>Rotational Con. (GHz)</b>	0.642546	0.6771913	0.9487325	0.5749996	0.975120
<b>H298</b>	-				
<b>6-31+g** tight PCM</b>	-593.331058	-593.326048	-442.845688	-593.3550315	-442.418426
<b>6-31g* tight</b>	-593.279439	-593.282047	-442.737851	-593.3082895	-442.381413
<b>G298</b>	-6.472538	-3.208959			
<b>6-31+g** tight PCM</b>	-593.383320	-593.378119	-442.890835	-593.4059685	-442.463054
<b>6-31g* tight</b>	-593.331701	-593.334118	-442.782998	-593.3592265	-442.426041



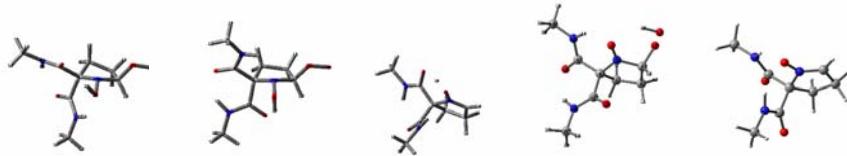
Compound	DEPMPO-H-OO cis	DEPMPO-H- OO trans	DEPMPO-H-OO cis	DEPMPO-H-OO trans	DEPMPO-H	DEPMPO-OOH posdepO2Hnewb.l og	DEPMPO-3
file	DEPMPO-H-O2- trans.log	DEPMPO-H- O2-cis.log	DEPMPO-H-O2- cis-b.log	DEPMPO-H-O2- trans-b.log	DEPMPO-H.log		dep-3.log
E 6-31+g** tight PCM	-1201.775226	-1201.775677	-1201.77439	-1201.777038	-1051.275339	-1201.8034220	-1050.844784
E 6-31g*	-1201.718848	-1201.719975	-1201.711276	-1201.718912	-1051.177801	-1201.7499825	-1050.798529
ZPE (raw)	0.296541	0.296340	0.295969	0.296193	0.290239	0.2973320	0.277828
Therm Corr to H (raw)	0.317601	0.317605	0.317179	0.317463	0.308985	0.3182380	0.296395
Therm Corr to G (raw)	0.245553	0.244185	0.243473	0.243985	0.24309	0.2468640	0.230716
H (raw)							-1050.502134
G (raw)							-1050.567813
ZPE (scaled)	0.290788	0.290591	0.290227	0.290447	0.284608	0.2915638	0.272438
Electronic State	2-A	2-A	2-A	2-A	1-A	2-A	
s2 6-31g*	0.754200	0.754300	0.7543	0.7543	0	0.7546000	0.000000
Symmetry	C1	C1	C1	C1	C1	C1	C01
N Imag	0.000000	0.000000	#NAME?	0.000000	0	0.0000000	0.000000
Rotational Con. (GHz)	0.664134	0.605048	0.6620344	0.632996	0.5982473	0.6347177	0.650529
Rotational Con. (GHz)	0.298724	0.301407	0.2983201	0.2967351	0.5221811	0.3002543	0.483010
Rotational Con. (GHz)	0.259536	0.236517	0.2579806	0.240893	0.3476093	0.2399654	0.3335952
H298							
6-31+g** tight PCM	-1201.463378	-1201.463821	-1201.462953	-1201.465321	-1050.971985	-1201.4909522	-1050.553779
6-31g* tight	-1201.407000	-1201.408119	-1201.399839	-1201.407195	-1050.874446	-1201.4375127	-1050.507524
G298	-9.648748	-10.787741	-10.422407	-11.765494	94438.640004		
6-31+g** tight PCM	-1201.535426	-1201.537241	-1201.536659	-1201.538799	-1051.037880	-1201.5623262	-1050.619458
6-31g* tight	-1201.479048	-1201.481539	-1201.473545	-1201.480673	-1050.940341	-1201.5088867	-1050.573203



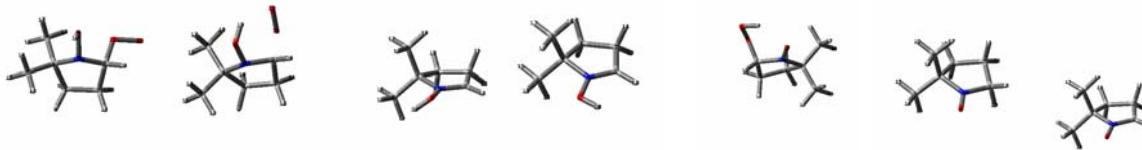
<b>Compound</b>	<b>DEPO-H-O2</b>	<b>DEPO-H-O2</b>	<b>DEPO-H</b>	<b>DiEtMPO-OOH</b>	<b>DEPO Nitrone</b>
<b>file</b>	<b>DEPO-H-O2.log</b>	<b>DEPO-H-O2-b.log</b>	<b>DEPO-H.log</b>	<b>posDEPO-HO2TSb.log</b>	<b>DEPOb.log</b>
<b>E 6-31+g** tight PCM</b>	-971.901834	-971.893598	-821.397879	-971.9228910	-820.962262
<b>E 6-31g*</b>	-971.844574	-971.8375126	-821.2965018	-971.8653170	-820.91136
<b>ZPE (raw)</b>	0.272012	0.272029	0.265414	0.2724210	0.252889
<b>Therm Corr to H (raw)</b>	0.292355	0.292243	0.283311	0.2925880	0.270692
<b>Therm Corr to G (raw)</b>	0.221873	0.221659	0.219195	0.2225580	0.206682
<b>H (raw)</b>					
<b>G (raw)</b>					
<b>ZPE (scaled)</b>	0.266735	0.266752	0.260265	0.2671360	0.247983
<b>Electronic State</b>	2-A	2-A	1-A	2-A	1-A
<b>s2 6-31g*</b>	0.754000	0.754	0	0.7542000	0
<b>Symmetry</b>	C1	C1	C1	C1	C1
<b>N Imag</b>	0.000000	0	0	0.0000000	0.000000
<b>Rotational Con. (GHz)</b>	0.481719	0.507707	0.7664617	0.4601682	0.69608
<b>Rotational Con. (GHz)</b>	0.344161	0.3368519	0.3622525	0.3757929	0.40056
<b>Rotational Con. (GHz)</b>	0.245097	0.250146	0.3143297	0.2520042	0.314700
<b>H298</b>					
<b>6-31+g** tight PCM</b>	-971.614756	-971.606632	-821.119717	-971.6355880	-820.696476
<b>6-31g* tight</b>	-971.557496	-971.550547	-821.018340	-971.5780140	-820.645574
<b>G298</b>	-12.070146	-7.036472			
<b>6-31+g** tight PCM</b>	-971.685238	-971.677216	-821.183833	-971.7056180	-820.760486
<b>6-31g* tight</b>	-971.627978	-971.621131	-821.082456	-971.6480440	-820.709584



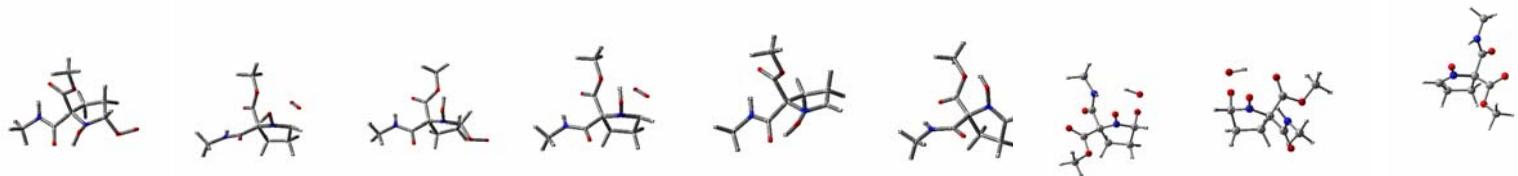
Compound	H- OO cis DiMAMPO-H- O2-cis.log	DiMAMPO-H- OO trans DiMAMPO-H- O2-trans.log	DiMAMPO-H- OO-2 cis DiMAMPO-H- O2-cis-b.log	DiMAMPO-H- OO-2 trans DiMAMPO-H- O2-trans-b.log	DiMAMPO-H DiMAMPO-H.log	DiMAMPO-OOH DiMAMPO-O2H- B3LYP_pos.log	diMAMPO diMAMPO_3.lo g
E 6-31+g** tight PCM	-724.144312	-724.144356	-724.13753	-724.138786	-573.653702	-724.1657820	-573.20707
E 6-31g*	-724.090818	-724.092880	-724.0726232	-724.0803471	-573.556366	-724.1179248	-573.160583
ZPE (raw)	0.241111	0.241654	0.240154	0.240584	0.234747	0.2419010	0.221908
Therm Corr to H (raw)	0.257381	0.257768	0.256691	0.257026	0.248387	0.2578940	0.235679
Therm Corr to G (raw)	0.197718	0.198879	0.196069	0.196789	0.196106	0.1989930	0.182679
H (raw)							
G (raw)							
ZPE (scaled)	0.236433	0.236966	0.235495	0.235917	0.230193	0.2372081	0.217603
Electronic State	2-A	2-A	2-A	2-A	1-A	2-A	1-A
s2 6-31g*	0.754300	0.754300	0.7543	0.7543	0.000000	0.7546000	0
Symmetry	C1	C1	C1	C1	C1	C1	C1
N Imag	0.000000	0.000000	0.000000	0	0.000000	0.0000000	0.000000
Rotational Con. (GHz)	1.262454	1.439639	1.2638162	1.4429955	1.506493	0.9376540	1.508731
Rotational Con. (GHz)	0.426369	0.434133	0.4203949	0.4242955	0.745759	0.5514136	0.718530
Rotational Con. (GHz)	0.397236	0.389598	0.3997656	0.3908227	0.607909	0.4961908	0.687513
H298							
6-31+g** tight PCM	-723.891609	-723.891276	-723.885498	-723.886427	-573.409869	-723.9125809	-572.975696
6-31g* tight	-723.838114	-723.839800	-723.820591	-723.827988	-573.312533	-723.8647237	-572.929209
G298	-4.362108	-3.667790	-1.129452	-1.471031	94433.353364		
6-31+g** tight PCM	-723.951272	-723.950165	-723.946120	-723.946664	-573.462150	-723.9714819	-573.028696
6-31g* tight	-723.897777	-723.898689	-723.881213	-723.888225	-573.364814	-723.9236247	-572.982209



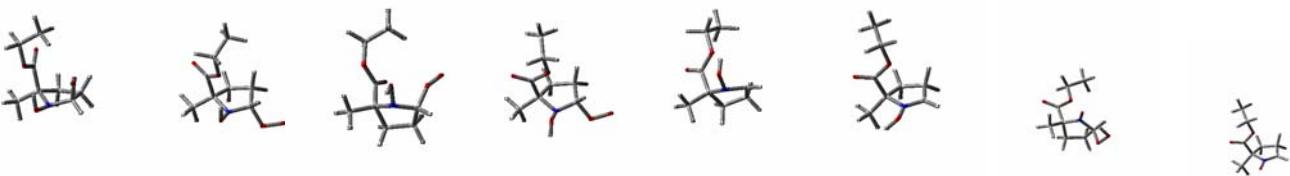
Compound	DiMAPO-H-OO DIMAPO-H- O2.log	DiMAPO-H- O2-b.log	DIMAPO-H DIMAPO-H.log	DiMAPO-OOH DiMAPO-O2H- B3LYP_neg.log	diMAPO diAmide_b3lyp- b.log
<b>E 6-31+g** tight PCM</b>	-853.554520	-853.559331	-703.054109	-853.5752370	-702.62004
<b>E 6-31g*</b>	-853.493261	-853.500073	-702.944767	-853.5154293	-702.569436
<b>ZPE (raw)</b>	0.240775	0.241132	0.233686	0.2409970	0.221602
<b>Therm Corr to H (raw)</b>	0.258824	0.258870	0.249248	0.2590270	0.237143
<b>Therm Corr to G (raw)</b>	0.193899	0.194860	0.191318	0.1939640	0.17825
<b>H (raw)</b>					
<b>G (raw)</b>					
<b>ZPE (scaled)</b>	0.236104	0.236454	0.229152	0.2363217	0.217303
<b>Electronic State</b>	2-A	2-A	1-A	2-A	1-A
<b>s2 6-31g*</b>	0.754200	0.754200	0.000000	0.7545000	0
<b>Symmetry</b>	C1	C1	C1	C1	C1
<b>N Imag</b>	0.000000	0.000000	0.000000	0.0000000	0.000000
<b>Rotational Con. (GHz)</b>	0.698873	0.659901	0.769657	0.6725997	0.7483062
<b>Rotational Con. (GHz)</b>	0.410314	0.449851	0.652692	0.4468623	0.6732812
<b>Rotational Con. (GHz)</b>	0.337024	0.328482	0.522087	0.3334124	0.5456517
<b>H298</b>					
<b>6-31+g** tight PCM</b>	-853.300367	-853.305139	-702.809395	-853.3208853	-702.387196
<b>6-31g* tight</b>	-853.239108	-853.245881	-702.700053	-853.2610776	-702.336592
<b>G298</b>	-9.913098	-12.333356			
<b>6-31+g** tight PCM</b>	-853.365292	-853.369149	-702.867325	-853.3859483	-702.446089
<b>6-31g* tight</b>	-853.304033	-853.309891	-702.757983	-853.3261406	-702.395485



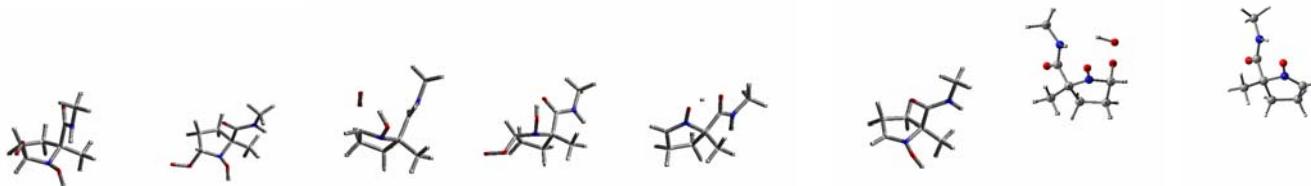
Compound	DMPO-H-OO- b	DMPO-O2-H- b.log	DMPO-H	DMPO-H-b DMPO-H-b- F.log	DMPO-OOH C-O oxdmopoOTS+freq .log	DMPO-H2 DMPO-H2- F.log	DMPO dmpo1.log
file	DMPO-H-O2.log		DMPO-H-F.log	DMPO-H-b- F.log	oxdmopoOTS+freq .log	DMPO-H2- F.log	
<b>E 6-31+g** tight PCM</b>	-516.141400	-516.135344	-365.645832	-365.650906	-516.1655410	-365.607374	-365.208275
<b>E 6-31g*</b>	-516.096085	-516.098122	-365.5444646	-365.5418852	-516.1253238	-365.519434	-365.1773173
<b>ZPE (raw)</b>	0.185138	0.185223	0.178782	0.178779	0.1859500	0.178653	0.166744
<b>Therm Corr to H (raw)</b>	0.196928	0.196735	0.188237	0.188314	0.1973390	0.187982	0.175674
<b>Therm Corr to G (raw)</b>	0.147518	0.148957	0.146618	0.146406	0.1499050	0.146235	0.134895
<b>H (raw)</b>					-515.9279850		-365.001643
<b>G (raw)</b>					-515.9754190		-365.042422
<b>ZPE (scaled)</b>	0.181546	0.181630	0.175314	0.175311	0.1823426	0.1751871	0.163509
<b>Electronic State</b>	2-A	2-A	1-A	1-A		1-A	
<b>s2 6-31g*</b>	0.754300	0.7546	0	0	0.7538000	0	0.000000
<b>Symmetry</b>	C1	C1	C1	C1	C1	C1	C01
<b>N Imag</b>	0.000000	0.000000	0	0.000000	0.0000000	0	0.000000
<b>Rotational Con. (GHz)</b>	2.083754	1.9039928	2.4640397	2.498307	-	2.577180	2.611353
<b>Rotational Con. (GHz)</b>	1.075983	1.2291736	2.2220507	2.2096885	-	2.158301	2.250094
<b>Rotational Con. (GHz)</b>	0.937951	1.025286	1.603907	1.607885	-	1.6300171	1.6682067
<b>H298</b>							
<b>6-31+g** tight PCM</b>	-515.948064	-515.942202	-365.461063	-365.466060	-515.9718094	-365.422858	-365.035836
<b>6-31g* tight</b>	-515.902749	-515.904980	-365.359696	-365.357040	-515.9315922	-365.334918	-365.004878
<b>G298</b>	-4.603011	0.099138	3.316979		-94450.5719720	-27.210973	
<b>6-31+g** tight PCM</b>	-515.997474	-515.989980	-365.502682	-365.507968	-516.0192434	-365.464605	-365.076615
<b>6-31g* tight</b>	-515.952159	-515.952758	-365.401315	-365.398948	-515.9790262	-365.376665	-365.045657



Compound	EMAPO-H-OO cis	EMAPO-H-OO trans	EMAPO-H-OO cis	EMAPO-H-OO trans	EMAPO-H	EMAPO-H-b	EMAPO-OOH cis	EMAPO-OOH- trans	EMAPO
file	EMAPO-H-O2- cis.log	EMAPO-H-O2- trans.log	EMAPO-H-O2- cis-b.log	EMAPO-H-O2- trans-b.log	EMAPO-H.log	EMAPO-H- b.log	EMAPO-O2H- B3LYP_neg.log	EMAPO-HO2- B3LYP-trans- pos.log	AMEST_b3lyp.1 og
<b>E 6-31+g** tight PCM</b>	-873.406176	-873.400711	-873.401486	-873.399418	-722.905353	-722.899187	-873.4234290	-873.4294970	-722.470809
<b>E 6-31g*</b>	-873.346094	-873.344284	-873.3370553	-873.3405968	-722.8015623	722.7934984	-873.3674183	-873.3744579	-722.4241912
<b>ZPE (raw)</b>	0.227777	0.228026	0.22735	0.227765	0.221355	0.221348	0.2282570	0.2285670	0.208944
<b>Therm Corr to H (raw)</b>	0.245731	0.245905	0.245376	0.24575	0.23672	0.236981	0.2459700	0.2461210	0.224266
<b>Therm Corr to G (raw)</b>	0.181530	0.182061	0.179806	0.181299	0.179397	0.178929	0.1828790	0.1833590	0.166673
<b>H (raw)</b>									
<b>G (raw)</b>									
<b>ZPE (scaled)</b>	0.223358	0.223602	0.222939	0.223346	0.217061	0.217054	0.2238288	0.2241328	0.204890
<b>Electronic State</b>	2-A	2-A	2-A	2-A	1-A	1-A	2-A	2-A	1-A
<b>s2 6-31g*</b>	0.754200	0.754200	0.7542	0.7542	0	0	0.7544000	0.7543000	0
<b>Symmetry</b>	C1	C1	C1	C1	C1	C1	C1	C1	C1
<b>N Imag</b>	0.000000	0.000000	0	0	0	0	0.0000000	0.0000000	0.000000
<b>Rotational Con. (GHz)</b>	0.699913	0.758253	0.6946447	0.7554424	0.8491888	0.8008422	0.6971941	0.6902058	0.8696075
<b>Rotational Con. (GHz)</b>	0.429841	0.477164	0.4378778	0.4816852	0.6314746	0.6829849	0.5029197	0.4738116	0.6410939
<b>Rotational Con. (GHz)</b>	0.331876	0.398916	0.3267838	0.3908124	0.5085944	0.4920138	0.3883797	0.3951368	0.5181203
<b>H298</b>									
<b>6-31+g** tight PCM</b>	-873.164864	-873.159230	-873.160521	-873.158087	-722.672927	-722.666500	-873.1818872	-873.1878102	-722.250597
<b>6-31g* tight</b>	-873.104782	-873.102802	-873.096090	-873.099265	-722.569137	-722.560812	-873.1258765	-873.1327711	-722.203979
<b>G298</b>	-10.444636	-6.685121	-8.578245	-6.348736	94439.435892	6			
<b>6-31+g** tight PCM</b>	-873.229065	-873.223074	-873.226091	-873.222538	-722.730250	-722.724552	-873.2449782	-873.2505722	-722.308190
<b>6-31g* tight</b>	-873.168983	-873.166646	-873.161660	-873.163716	-722.626460	-722.618864	-873.1889675	-873.1955331	-722.261572



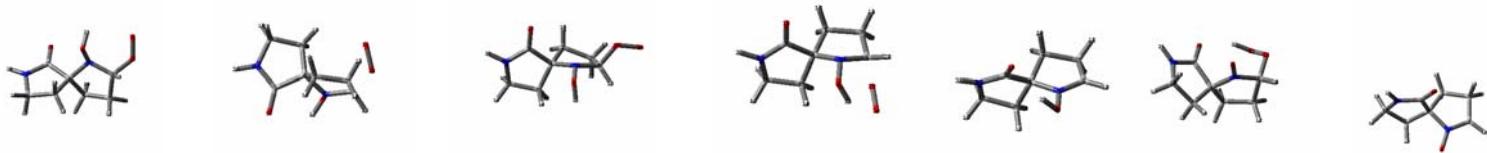
Compound	EMPO-H-OO cis file	EMPO-H-OO trans	EMPO-H-O2- cis.log	EMPO-H-OO cis EMPO-H-O2- trans.log	EMPO-H-OO trans	EMPO-H-OO trans-b.log	EMPO-H	EMPO-H-b EMPO-H- b.log	EMPO-OOH posempO2Hdsp.lo g	EMPO-1 empocis.log
E 6-31+g** tight PCM	-744.020012	-744.020582	-744.022337	-744.026175	-593.519758	-593.52003	-	-	-744.0464210	-593.088055
E 6-31g*	-743.974888	-743.970664	-743.9686778	-743.9721409	-593.4218746	593.4135061	-	-	-743.9974642	-593.0478221
ZPE (raw)	0.229120	0.228972	0.228828	0.228886	0.222445	0.222005	0.2291990	0.223456	0.210235	
Therm Corr to H (raw)	0.244760	0.244664	0.244726	0.244793	0.236	0.235816	0.2450910	0.223456		
Therm Corr to G (raw)	0.187109	0.186022	0.185803	0.185547	0.182894	0.182548	0.1848420	0.171267		
H (raw)										-592.824366
G (raw)										-592.876555
ZPE (scaled)	0.224675	0.224530	0.224389	0.224446	0.218130	0.217698	0.2247525	0.206156		
Electronic State	2-A	2-A	2-A	2-A	1-A	1-A	2-A			
s2 6-31g*	0.754400	0.754200	0.7542	0.7542	0	0	0.7545000	0.000000		
Symmetry	C1	C1	C1	C1	C1	C1	C1	C1	C01	
N Imag	0.000000	0.000000	0	0	0.000000	0	0.0000000	0.000000		
Rotational Con. (GHz)	0.863491	0.997496	0.8498426	1.0102369	1.5184164	1.3444718	1.0129373	1.397008		
Rotational Con. (GHz)	0.697837	0.495740	0.6768697	0.4958833	0.6669127	0.7192755	0.4838898	0.726683		
Rotational Con. (GHz)	0.554890	0.431237	0.5296889	0.4239538	0.6045919	0.6517208	0.4174045	0.6549509		
H298										
6-31+g** tight PCM	-743.779697	-743.780360	-743.782050	-743.785822	-593.288073	-593.288521	-743.8057765	-592.868678		
6-31g* tight	-743.734573	-743.730442	-743.728391	-743.731788	-593.190190	-593.181997	-743.7568196	-592.828445		
G298	-8.784189	-9.822170	-11.059121	-13.628851						
6-31+g** tight PCM	-743.837348	-743.839002	-743.840973	-743.845068	-593.341179	-593.341789	-743.8660255	-592.920867		
6-31g* tight	-743.792224	-743.789084	-743.787314	-743.791034	-593.243296	-593.235265	-743.8170686	-592.880634		



Compound	MAMPO-H-OO cis	MAMPO-H-OO trans	MAMPO-H-OO cis	MAMPO-H-OO trans	MAMPO-H	MAMPO-H-b	MAMPO-OOH	MAMPO
file	MAMPO-H-O2- cis.log	MAMPO-H- O2-trans.log	MAMPO-H-O2- cis-b.log	MAMPO-H-O2- trans-b.log	MAMPO-H.log	MAMPO-H-b.log	MAMPO-O2H- B3LYP_neg.log	mampo.log
<b>E 6-31+g** tight PCM</b>	-684.850103	-684.849739	-684.840576	-684.849165	-534.34855	-534.356902	-684.8685890	-533.916533
<b>E 6-31g*</b>	-684.792091	-684.788902	-684.7917695	-684.7924313	-534.234429	534.2513091	-684.8177671	-533.8765506
<b>ZPE (raw)</b>	0.212815	0.212672	0.212736	0.213097	0.206057	0.206565	0.2135770	0.194399
<b>Therm Corr to H (raw)</b>	0.227768	0.227772	0.227469	0.227848	0.218876	0.218823	0.2281580	0.206546
<b>Therm Corr to G (raw)</b>	0.171071	0.169413	0.17166	0.171066	0.168441	0.169458	0.1731110	0.157121
<b>H (raw)</b>								
<b>G (raw)</b>								
<b>ZPE (scaled)</b>	0.208686	0.208546	0.208609	0.208963	0.202059	0.202558	0.2094336	0.190628
<b>Electronic State</b>	2-A	2-A	2-A	2-A	1-A	1-A	2-A	
<b>s2 6-31g*</b>	0.754200	0.754200	0.7546	0.7542	0	0	0.7544000	0
<b>Symmetry</b>	C1	C1	C1	C1	C1	C1	C1	C1
<b>N Imag</b>	0.000000	0.000000	0	0	0	0	0.0000000	0.000000
<b>Rotational Con. (GHz)</b>	0.941087	1.487366	0.9534471	1.5327854	1.6654899	1.8066517	1.0069100	1.6022635
<b>Rotational Con. (GHz)</b>	0.797915	0.503587	0.8232508	0.493895	0.862127	0.8546722	0.7887181	0.9445682
<b>Rotational Con. (GHz)</b>	0.636877	0.491793	0.6678084	0.4873138	0.8208847	0.7198606	0.6379280	0.8232683
<b>H298</b>								
<b>6-31+g** tight PCM</b>	-684.626464	-684.626093	-684.617234	-684.625451	-534.133672	-534.142086	-684.6445744	-533.713758
<b>6-31g* tight</b>	-684.568451	-684.565256	-684.568428	-684.568717	-534.019551	-534.036494	-684.5937525	-533.673776
<b>G298</b>	-5.985970	-6.796226	0.362878	-5.403937	94439.586192	6		
<b>6-31+g** tight PCM</b>	-684.683161	-684.684452	-684.673043	-684.682233	-534.184107	-534.191451	-684.6996214	-533.763183
<b>6-31g* tight</b>	-684.625148	-684.623615	-684.624237	-684.625499	-534.069986	-534.085859	-684.6487995	-533.723201



Compound	MSMPO-H-OO cis MSMPO-H-O2- cis.log	MSMPO-H-OO trans MSMPO-H- O2-trans.log	MSMPO-H-OO cis MSMPO-H-O2- cis-b.log	MSMPO-H-OO trans MSMPO-H-O2- trans-b.log	MSMPO-H MSMPO-H.log	MSMPO-OOH negmsmpO2H.I og	MSMPO so2ch3.log
E 6-31+g** tight PCM	-1064.728020	-1064.727139	-1064.723362	-1064.724393	-914.217058	-1064.7477060	-913.786021
E 6-31g*	-1064.665757	-1064.670691	-1064.652931	-1064.661435	-914.109970	-1064.6897053	-913.7353655
ZPE (raw)	0.195181	0.195385	0.194422	0.194943	0.188800	0.1956660	0.176304
Therm Corr to H (raw)	0.210301	0.210321	0.209683	0.210044	0.201239	0.2105650	0.188712
Therm Corr to G (raw)	0.153072	0.154287	0.152042	0.153326	0.152172	0.1543480	0.139196
H (raw)							-913.546653
G (raw)							-913.596170
ZPE (scaled)	0.191394	0.191595	0.190650	0.191161	0.185137	0.1918701	0.172884
Electronic State	2-A	2-A	2-A	2-A	1-A	2-A	
s2 6-31g*	0.754200	0.754200	0.7542	0.7542	0.000000	0.7545000	0.000000
Symmetry	C1	C1	C1	C1	C1	C1	C0
N Imag	0.000000	0.000000	0	0	#NAME?	0.0000000	0.000000
Rotational Con. (GHz)	1.253769	1.418060	1.2211848	1.4081834	1.412762	1.3465703	1.427094
Rotational Con. (GHz)	0.493003	0.493328	0.5035461	0.4893491	0.921695	0.5072307	0.933019
Rotational Con. (GHz)	0.480147	0.463619	0.4894565	0.4574832	0.836459	0.4747348	0.838985
H298							
6-31+g** tight PCM	-1064.521506	-1064.520608	-1064.517451	-1064.518131	-914.019482	-1064.5409369	-913.600729
6-31g* tight	-1064.459243	-1064.464161	-1064.447020	-1064.455173	-913.912394	-1064.4829362	-913.550074
G298	-17.580175	-16.267399	-15.294331	-15.141914	94446.571431		
6-31+g** tight PCM	-1064.578735	-1064.576642	-1064.575092	-1064.574849	-914.068549	-1064.5971539	-913.650245
6-31g* tight	-1064.516472	-1064.520195	-1064.504661	-1064.511891	-913.961461	-1064.5391532	-913.599590



Compound	TAMPO-H-OO cis	TAMPO-H-OO trans	TAMPO-H-OO cis	TAMPO-H-OO trans	TAMPO-H	TAMPO-OOH	TAMPO
file	TAMPO-H-O2-cis.log	TAMPO-H-O2-trans.log	TAMPO-H-O2-cis-b.log	TAMPO-H-O2-trans-b.log	TAMPO-H.log	poslam2.log	lam.log
E 6-31+g** tight PCM	-683.651763	-683.649364	-683.649197	-683.64652	-533.149512	-683.6763890	-532.716449
E 6-31g*	-683.582462	-683.581666	-683.5717943	-683.581272	-533.032461	-683.6136914	-532.6611844
ZPE (raw)	0.192350	0.192495	0.191786	0.192266	0.186493	0.1938610	0.173838
Therm Corr to H (raw)	0.205349	0.205521	0.204848	0.205154	0.196798	0.2061330	0.184087
Therm Corr to G (raw)	0.153211	0.153290	0.152298	0.1533	0.152182	0.1563900	0.139172
H (raw)							-532.477097
G (raw)							-532.522013
ZPE (scaled)	0.188618	0.188761	0.188065	0.188536	0.182875	0.1901001	0.170466
Electronic State	2-A	2-A	2-A	2-A	1-A	2-A	
s2 6-31g*	0.754100	0.754200	0.7542	0.7546	0.000000	0.7544000	0.000000
Symmetry	C1	C1	C1	C1	C1	C1	C01
N Imag	0.000000	0.000000	0	0	0.000000	0.0000000	0.000000
Rotational Con. (GHz)	1.474136	1.358752	1.5938069	1.3445681	1.731033	1.3703243	
Rotational Con. (GHz)	0.589981	0.659671	0.5329543	0.6500256	1.077539	0.7182703	
Rotational Con. (GHz)	0.550805	0.610186	0.5155723	0.6099974	0.887328	0.6558146	
H298							
6-31+g** tight PCM	-683.450146	-683.447577	-683.448070	-683.445096	-532.956332	-683.4740169	-532.535734
6-31g* tight	-683.380845	-683.379879	-683.370667	-683.379848	-532.839281	-683.4113194	-532.480470
G298	-12.026612	-10.473409	-10.982473	-8.679709	94441.017868		
6-31+g** tight PCM	-683.502284	-683.499808	-683.500620	-683.496950	-533.000948	-683.5237599	-532.580649
6-31g* tight	-683.432983	-683.432110	-683.423217	-683.431702	-532.883897	-683.4610624	-532.525385



Compound	TFMPO-H-O2-cis.log	TFMPO-H-OO trans	TFMPO-H-OO cis	TFMPO-H-O2-trans-b.log	TFMPO-H	TFMPO-H-b	TFMPO-OOH	TFMPO
file		TFMPO-H-O2-trans.log	TFMPO-H-O2-cis-b.log		TFMPO-H.log	TFMPO-H-b.log	tf_HO2TSfneg.log	tfmpo.log
E 6-31+g** tight PCM	-813.877708	-813.880675	-813.873477	-813.874883	-663.376518	-663.370312	-813.9008730	-662.941765
E 6-31g*	-813.814008	-813.818474	-813.8167798	-813.8145165	-663.247552	-663.2538957	-813.8447617	-662.8940932
ZPE (raw)	0.162286	0.162277	0.162051	0.162013	0.155451	0.155885	0.1629560	0.143603
Therm Corr to H (raw)	0.175846	0.175858	0.175704	0.175664	0.166951	0.167141	0.1762980	0.154463
Therm Corr to G (raw)	0.122985	0.122565	0.12214	0.121745	0.119798	0.120458	0.1234480	0.108489
H (raw)								-662.73963
G (raw)								-662.785604
ZPE (scaled)	0.159138	0.159129	0.158907	0.158870	0.152435	0.152861	0.1597947	0.140817
Electronic State	2-A	2-A	2-A	2-A	1-A	1-A	2-A	
s2 6-31g*	0.754200	0.754100	0.7544	0.7542	0	0	0.7544000	0.000000
Symmetry	C1	C1	C1	C1	C1	C1	C1	C01
N Imag	0.000000	0.000000	0	0	0	0	0.0000000	0.000000
Rotational Con. (GHz)	1.190726	1.419561	1.161028	1.422909	1.4981429	1.5105439	1.4586532	
Rotational Con. (GHz)	0.677428	0.565677	0.698811	0.563258	1.0926285	1.0782299	0.5804589	
Rotational Con. (GHz)	0.655708	0.539832	0.6721374	0.5361988	0.9619388	0.951052	0.5331642	
H298								
6-31+g** tight PCM	-813.705010	-813.707965	-813.700917	-813.702362	-663.212583	-663.206195	-813.7277363	-662.790088
6-31g* tight	-813.641311	-813.645765	-813.644220	-813.641996	-663.083617	-663.089779	-813.6716250	-662.742416
G298	-10.018565	-12.143830	-7.890957	-9.020639	94439.009821	94443.313018		
6-31+g** tight PCM	-813.757871	-813.761258	-813.754481	-813.756281	-663.259736	-663.252878	-813.7805863	-662.836062
6-31g* tight	-813.694172	-813.699058	-813.697784	-813.695915	-663.130770	-663.136462	-813.7244750	-662.788390



<b>Compound</b>	<b>H<sub>2</sub>O</b>	<b>H<sub>3</sub>O<sup>+</sup></b>	<b>Superoxide Radical</b>
<b>file</b>	H2O.log	H3Ob.log	o2.log
<b>E 6-31+g** tight PCM</b>	-76.444738	-76.845424	-150.465075
<b>E 6-31g*</b>	-76.40895332	-76.6890842	-150.2996938
<b>ZPE (raw)</b>	0.021168	0.034304	0.002761
<b>Therm Corr to H (raw)</b>	0.024947	0.038139	0.006082
<b>Therm Corr to G (raw)</b>	0.003501	0.015147	-0.017041
<b>H (raw)</b>			-150.293612
<b>G (raw)</b>			-150.316735
<b>ZPE (scaled)</b>	0.020757	0.033639	0.002707
<b>Electronic State</b>	1-A1	-	
<b>s2 6-31g*</b>	0	0	0.7528
<b>Symmetry</b>	C2V	-	C01
<b>N Imag</b>	0	0.000000	0
<b>Rotational Con. (GHz)</b>	787.90918	323.8423659	1.63425
<b>Rotational Con. (GHz)</b>	432.30875	323.5417689	0.75785
<b>Rotational Con. (GHz)</b>	279.14688	186.8424633	0.66048
<b>H298</b>			
<b>6-31+g** tight PCM</b>	-76.420202	-76.807950	-150.459047
<b>6-31g* tight</b>	-76.384417	-76.651611	-150.293665
<b>G298</b>			
<b>6-31+g** tight PCM</b>	-76.441648	-76.830942	-150.48217
<b>6-31g* tight</b>	-76.405863	-76.674603	-150.316788

**Table S9.** Thermodynamic data for nitrones and nitrone-H<sup>+</sup> at the PCM/B3LYP/6-311+G\*//B3LYP/6-311+G\* level at 298 K.



Compound	DMPO-H	DMPO	Pagas
file	DMPO-H-pka-a.log	DMPO-pka.log	217.2523014
E 6-311+g* tight (PCM)	-365.7289423	-365.2930541	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-365.6269732	-365.2687237	48.71903311
ZPE (raw)	0.177865	0.165591	
Therm Corr to H (raw)	0.187341	0.174526	
Therm Corr to G (raw)	0.1457	0.133778	
H (raw)			
G (raw)			
ZPE (scaled)	0.174414	0.162379	
Electronic State	1-A	1-A	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	2.4588252	2.6009879	
Rotational Con. (GHz)	2.2309934	2.2587957	
Rotational Con. (GHz)	1.6042864	1.6679096	
H298			
6-311+g* tight (PCM)	-365.545052	-365.121741	
6-311+g*	-365.443083	-365.097410	
G298			
6-311+g* tight (PCM)	-365.586693	-365.162489	
6-311+g*	-365.484724	-365.138158	



Compound	DMPO-H-b	DMPO	Pagas
file	DMPO-H-pka-b.log	DMPO-pka.log	215.6416301
E 6-311+g* tight (PCM)	-365.7247174	-365.2930541	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-365.6243574	-365.2687237	47.7093377
ZPE (raw)	0.177815	0.165591	
Therm Corr to H (raw)	0.187418	0.174526	
Therm Corr to G (raw)	0.145254	0.133778	
H (raw)			
G (raw)			
ZPE (scaled)	0.174365	0.162379	
Electronic State	1-A	1-A	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	2.4984809	2.6009879	
Rotational Con. (GHz)	2.2152771	2.2587957	
Rotational Con. (GHz)	1.609241	1.6679096	
H298			
6-311+g* tight (PCM)	-365.540749	-365.121741	
6-311+g*	-365.440389	-365.097410	
G298			
6-311+g* tight (PCM)	-365.582913	-365.162489	
6-311+g*	-365.482553	-365.138158	



<b>Compound</b>	<b>CPCOMPO-H</b>	<b>CPCOMPO</b>	<b>Pagas</b>
file	CPCOMPO-H-pka.log	CPCOMPO-pka.log	211.8167076
<b>E 6-311+g* tight (PCM)</b>	-553.1407667	-552.7051849	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-553.0190606	-552.6691027	53.72978118
<b>ZPE (raw)</b>	0.172823	0.160171	
<b>Therm Corr to H (raw)</b>	0.183154	0.170257	
<b>Therm Corr to G (raw)</b>	0.138269	0.12545	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.169470	0.157064	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	1.7535382	1.7782094	
<b>Rotational Con. (GHz)</b>	1.0544028	1.0436075	
<b>Rotational Con. (GHz)</b>	0.8996789	0.9733274	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-552.960965	-552.538035	
<b>6-311+g*</b>	-552.839259	-552.501953	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-553.005850	-552.582842	
<b>6-311+g*</b>	-552.884144	-552.546760	



<b>Compound</b>	<b>AMPO-H</b>	<b>AMPO</b>	<b>Pagas</b>
file	AMPO-H-pka-w.log	AMPO-pka.log	218.1214836
<b>E 6-311+g* tight (PCM)</b>	-495.1768211	-494.733661	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-495.060451	-494.7006232	52.29184505
<b>ZPE (raw)</b>	0.177479	0.165008	
<b>Therm Corr to H (raw)</b>	0.188159	0.175478	
<b>Therm Corr to G (raw)</b>	0.143007	0.130502	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.174036	0.161807	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	1.90646	1.7595215	
<b>Rotational Con. (GHz)</b>	1.28889	1.3696257	
<b>Rotational Con. (GHz)</b>	1.00572	1.1116692	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-494.992105	-494.561384	
<b>6-311+g*</b>	-494.875735	-494.528346	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-495.037257	-494.606360	
<b>6-311+g*</b>	-494.920887	-494.573322	



<b>Compound</b>	<b>CPPO-H</b>	<b>CPPO</b>	<b>Pgas</b>
file	CPPO-H-pka.log	CPPO-pka.log	218.406946
<b>E 6-311+g* tight (PCM)</b>	-443.1563554	-442.7189179	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-443.0575147	-442.6972948	48.45479953
<b>ZPE (raw)</b>	0.214952	0.202545	
<b>Therm Corr to H (raw)</b>	0.225389	0.21246	
<b>Therm Corr to G (raw)</b>	0.180339	0.167941	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.210782	0.198616	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	2.18157	2.2603559	
<b>Rotational Con. (GHz)</b>	1.1329712	1.1561797	
<b>Rotational Con. (GHz)</b>	0.9494354	0.9765595	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-442.935136	-442.510387	
<b>6-311+g*</b>	-442.836296	-442.488764	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-442.980186	-442.554906	
<b>6-311+g*</b>	-442.881346	-442.533283	



<b>Compound</b>	<b>EMPO-H</b>	<b>EMPO</b>	<b>Pagas</b>
<b>file</b>	EMPO-H-pka-F.log	EMPO-pka.log	216.4385761
<b>E 6-311+g* tight (PCM)</b>	-593.6685922	-593.2396053	$\Delta\Delta G_{\text{solv}}$
<b>E 6-311+g*</b>	-593.5612914	-593.2046005	45.36641301
<b>ZPE (raw)</b>	0.22069	0.208683	
<b>Therm Corr to H (raw)</b>	0.234603	0.222	
<b>Therm Corr to G (raw)</b>	0.180781	0.169388	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.216409	0.204635	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	#NAME?	
<b>Rotational Con. (GHz)</b>	1.3302328	1.3853371	
<b>Rotational Con. (GHz)</b>	0.719484	0.7238928	
<b>Rotational Con. (GHz)</b>	0.6577108	0.6583515	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-593.438271	-593.021654	
<b>6-311+g*</b>	-593.330970	-592.986649	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-593.492093	-593.074266	
<b>6-311+g*</b>	-593.384792	-593.039261	



Compound	DEPO-H	DEPO	Pagas
file	DEPO-H-pka.log	DEPO-pka.log	226.6027655
E 6-311+g* tight (PCM)	-821.6171913	-821.1812073	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-821.5074948	-821.1337992	39.0865778
ZPE (raw)	0.263978	0.251148	
Therm Corr to H (raw)	0.281946	0.268964	
Therm Corr to G (raw)	0.217719	0.205106	
H (raw)			
G (raw)			
ZPE (scaled)	0.258857	0.246276	
Electronic State	1-A	1-A	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	0.7716245	0.6953258	
Rotational Con. (GHz)	0.3607257	0.4010782	
Rotational Con. (GHz)	0.3132359	0.3140745	
H298			
6-311+g* tight (PCM)	-821.340366	-820.917116	
6-311+g*	-821.230670	-820.869707	
G298			
6-311+g* tight (PCM)	-821.404593	-820.980974	
6-311+g*	-821.294897	-820.933565	



<b>Compound</b>	<b>DIMAPO-H</b>	<b>DIMAPO</b>	<b>Pagas</b>
file	DIMAPO-H-pka.log	DIMAPO-pka.log	220.9381135
E 6-311+g* tight (PCM)	-703.2427342	-702.802642	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-703.1236955	-702.7593977	47.56176127
ZPE (raw)	0.232724	0.220272	
Therm Corr to H (raw)	0.248427	0.235788	
Therm Corr to G (raw)	0.190047	0.177843	
H (raw)			
G (raw)			
ZPE (scaled)	0.228209	0.215999	
Electronic State	1-A	1-A	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	0.7731534	0.7606536	
Rotational Con. (GHz)	0.6505876	0.6664053	
Rotational Con. (GHz)	0.5179705	0.5421342	
H298			
6-311+g* tight (PCM)	-702.998822	-702.571127	
6-311+g*	-702.879783	-702.527883	
G298			
6-311+g* tight (PCM)	-703.057202	-702.629072	
6-311+g*	-702.938163	-702.585828	



<b>Compound</b>	<b>EMAPO-H</b>	<b>EMAPO</b>	<b>Pagas</b>
file	EMAPO-H-pka.log	EMAPO-pka.log	221.6577522
<b>E 6-311+g* tight (PCM)</b>	-723.1002939	-722.6675709	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-722.9885715	-722.6228495	42.04370063
<b>ZPE (raw)</b>	0.220304	0.207569	
<b>Therm Corr to H (raw)</b>	0.235767	0.222956	
<b>Therm Corr to G (raw)</b>	0.178212	0.165226	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.216030	0.203542	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	0.8543034	0.8726249	
<b>Rotational Con. (GHz)</b>	0.6295786	0.638213	
<b>Rotational Con. (GHz)</b>	0.5044517	0.5167378	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-722.868801	-722.448642	
<b>6-311+g*</b>	-722.757078	-722.403920	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-722.926356	-722.506372	
<b>6-311+g*</b>	-722.814633	-722.461650	



<b>Compound</b>	<b>MAMPO-H</b>	<b>MAMPO</b>	<b>Pagas</b>
<b>file</b>	MAMPO-H-pka.log	MAMPO-pka-b.log	212.2693352
<b>E 6-311+g* tight (PCM)</b>	-534.4784993	-534.0515931	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-534.3672201	-534.017291	48.30382074
<b>ZPE (raw)</b>	0.204912	0.193025	
<b>Therm Corr to H (raw)</b>	0.217834	0.205276	
<b>Therm Corr to G (raw)</b>	0.167161	0.155564	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.200937	0.189280	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	1.6724097	1.6059971	
<b>Rotational Con. (GHz)</b>	0.8572422	0.9416486	
<b>Rotational Con. (GHz)</b>	0.8198513	0.8237776	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-534.264641	-533.850062	
<b>6-311+g*</b>	-534.153361	-533.815760	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-534.315314	-533.899774	
<b>6-311+g*</b>	-534.204034	-533.865472	



<b>Compound</b>	<b>MSMPO-H</b>	<b>MSMPO</b>	<b>Pagas</b>
file	MSMPO-H-pka.log	MSMPO-pka.log	220.8619745
<b>E 6-311+g* tight (PCM)</b>	-914.3898856	-913.9475597	<b><math>\Delta\Delta G_{\text{solv}}</math></b>
<b>E 6-311+g*</b>	-914.2637644	-913.8992085	48.80144833
<b>ZPE (raw)</b>	0.187748	0.174909	
<b>Therm Corr to H (raw)</b>	0.200238	0.187399	
<b>Therm Corr to G (raw)</b>	0.151062	0.137611	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.184106	0.171516	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	1.4151097	1.4300269	
<b>Rotational Con. (GHz)</b>	0.9177769	0.9269387	
<b>Rotational Con. (GHz)</b>	0.8338581	0.8349185	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-914.193290	-913.763554	
<b>6-311+g*</b>	-914.067169	-913.715203	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-914.242466	-913.813342	
<b>6-311+g*</b>	-914.116345	-913.764991	



<b>Compound</b>	<b>TAMPO-H</b>	<b>TAMPO</b>	<b>Pgas</b>
<b>file</b>	TAMPO-H-pka.log	TAMPO-pka.log	218.3183855
<b>E 6-311+g* tight (PCM)</b>	-533.2784425	-532.8401858	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-533.1631901	-532.8027122	48.80698735
<b>ZPE (raw)</b>	0.185642	0.172828	
<b>Therm Corr to H (raw)</b>	0.196085	0.183121	
<b>Therm Corr to G (raw)</b>	0.151116	0.138059	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.182041	0.169475	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	1.7306996	1.7575137	
<b>Rotational Con. (GHz)</b>	1.0629103	1.0445416	
<b>Rotational Con. (GHz)</b>	0.895771	0.9653489	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-533.085959	-532.660418	
<b>6-311+g*</b>	-532.970707	-532.622944	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-533.130928	-532.705480	
<b>6-311+g*</b>	-533.015676	-532.668006	



<b>Compound</b>	<b>TFMPO-H</b>	<b>TFMPO</b>	<b>Pagas</b>
file	TFMPO-H-pka.log	TFMPO-pka.log	207.5308534
E 6-311+g* tight (PCM)	-663.5443854	-663.1173503	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-663.4314218	-663.0890273	53.11280129
ZPE (raw)	0.154145	0.142241	
Therm Corr to H (raw)	0.16587	0.153188	
Therm Corr to G (raw)	0.11795	0.106959	
H (raw)			
G (raw)			
ZPE (scaled)	0.151155	0.139482	
Electronic State	1-A	1-A	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	1.5048388	1.5440255	
Rotational Con. (GHz)	1.0801933	1.0858055	
Rotational Con. (GHz)	0.9525756	0.9618831	
H298			
6-311+g* tight (PCM)	-663.381506	-662.966922	
6-311+g*	-663.268542	-662.938599	
G298			
6-311+g* tight (PCM)	-663.429426	-663.013151	
6-311+g*	-663.316462	-662.984828	



Compound	DiMAMPO-H	DiMAMPO	Pagas
file	DiMAMPO-H-pka.log	DiMAMPO-pka.log	232.6605305
E 6-311+g* tight (PCM)	-573.7985079	-573.3490492	$\Delta\Delta G_{\text{solv}}$
E 6-311+g*	-573.6922074	-573.3085748	41.30646419
ZPE (raw)	0.23363	0.220511	
Therm Corr to H (raw)	0.247393	0.234292	
Therm Corr to G (raw)	0.194701	0.181366	
H (raw)			
G (raw)			
ZPE (scaled)	0.229098	0.216233	
Electronic State	1-A	1-A	
s2 6-31g*	0	0	
Symmetry	C1	C1	
N Imag	0.000000	0.000000	
Rotational Con. (GHz)	1.5105699	1.5168824	
Rotational Con. (GHz)	0.7434072	0.7159318	
Rotational Con. (GHz)	0.6081493	0.6866057	
H298			
6-311+g* tight (PCM)	-573.555647	-573.119035	
6-311+g*	-573.449347	-573.078561	
G298			
6-311+g* tight (PCM)	-573.608339	-573.171961	
6-311+g*	-573.502039	-573.131487	



<b>Compound</b>	<b>DEPMPO-H</b>	<b>DEPMPO</b>	<b>Pagas</b>
<b>file</b>	DEPMPO-H-pka_b.log	DEP-pka-cis-.log	223.3684615
<b>E 6-311+g* tight (PCM)</b>	-1051.49291	-1051.059847	<b>ΔΔGsolv</b>
<b>E 6-311+g*</b>	-1051.380287	-1051.01208	40.69793811
<b>ZPE (raw)</b>	0.288305	0.275816	
<b>Therm Corr to H (raw)</b>	0.307215	0.29439	
<b>Therm Corr to G (raw)</b>	0.240725	0.228975	
<b>H (raw)</b>			
<b>G (raw)</b>			
<b>ZPE (scaled)</b>	0.282712	0.270465	
<b>Electronic State</b>	1-A	1-A	
<b>s2 6-31g*</b>	0	0	
<b>Symmetry</b>	C1	C1	
<b>N Imag</b>	0.000000	0.000000	
<b>Rotational Con. (GHz)</b>	0.6131327	0.64213	
<b>Rotational Con. (GHz)</b>	0.5008902	0.49181	
<b>Rotational Con. (GHz)</b>	0.3435652	0.34679	
<b>H298</b>			
<b>6-311+g* tight (PCM)</b>	-1051.191288	-1050.770808	
<b>6-311+g*</b>	-1051.078665	-1050.723041	
<b>G298</b>			
<b>6-311+g* tight (PCM)</b>	-1051.257778	-1050.836223	
<b>6-311+g*</b>	-1051.145155	-1050.788456	