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Supporting Information

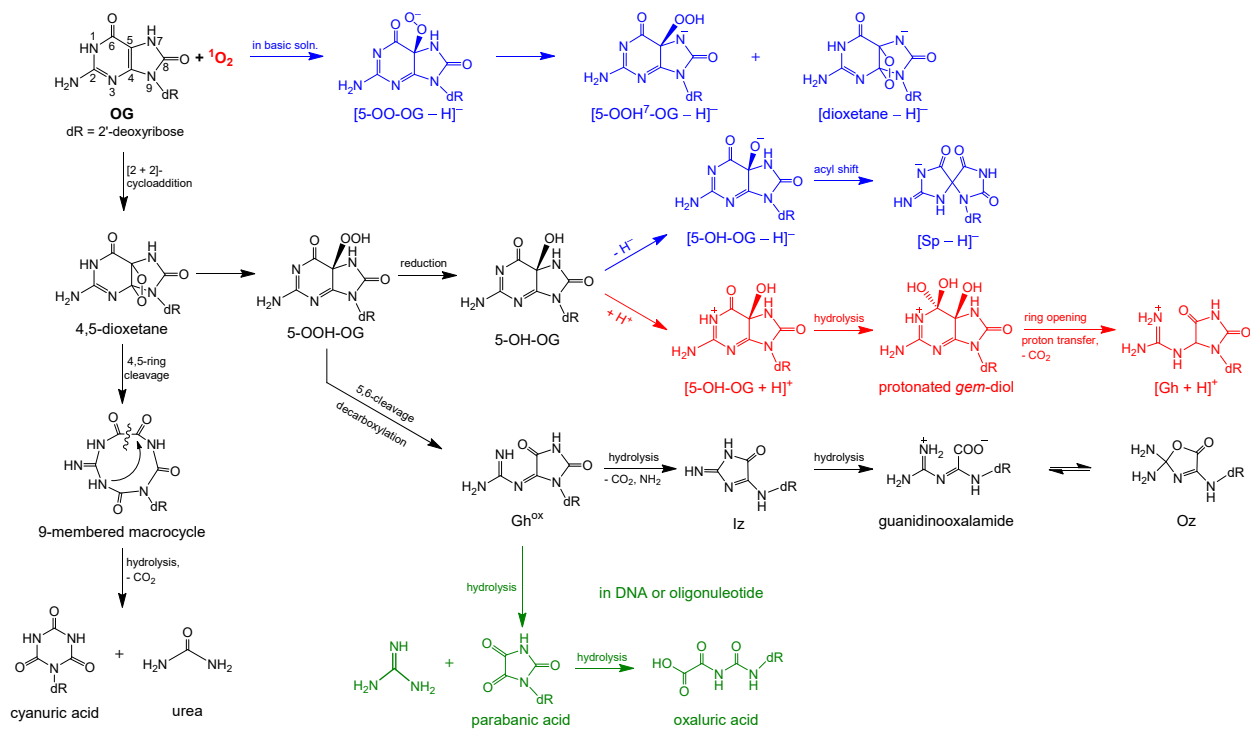
Effects of Intra-Base Pair Proton Transfer on Dissociation and Singlet Oxygenation of 9-Methyl-8-Oxoguanine–1-Methyl-Cytosine Base-Pair Radical Cations

May Myat Moe, Midas Tsai, and Jianbo Liu*

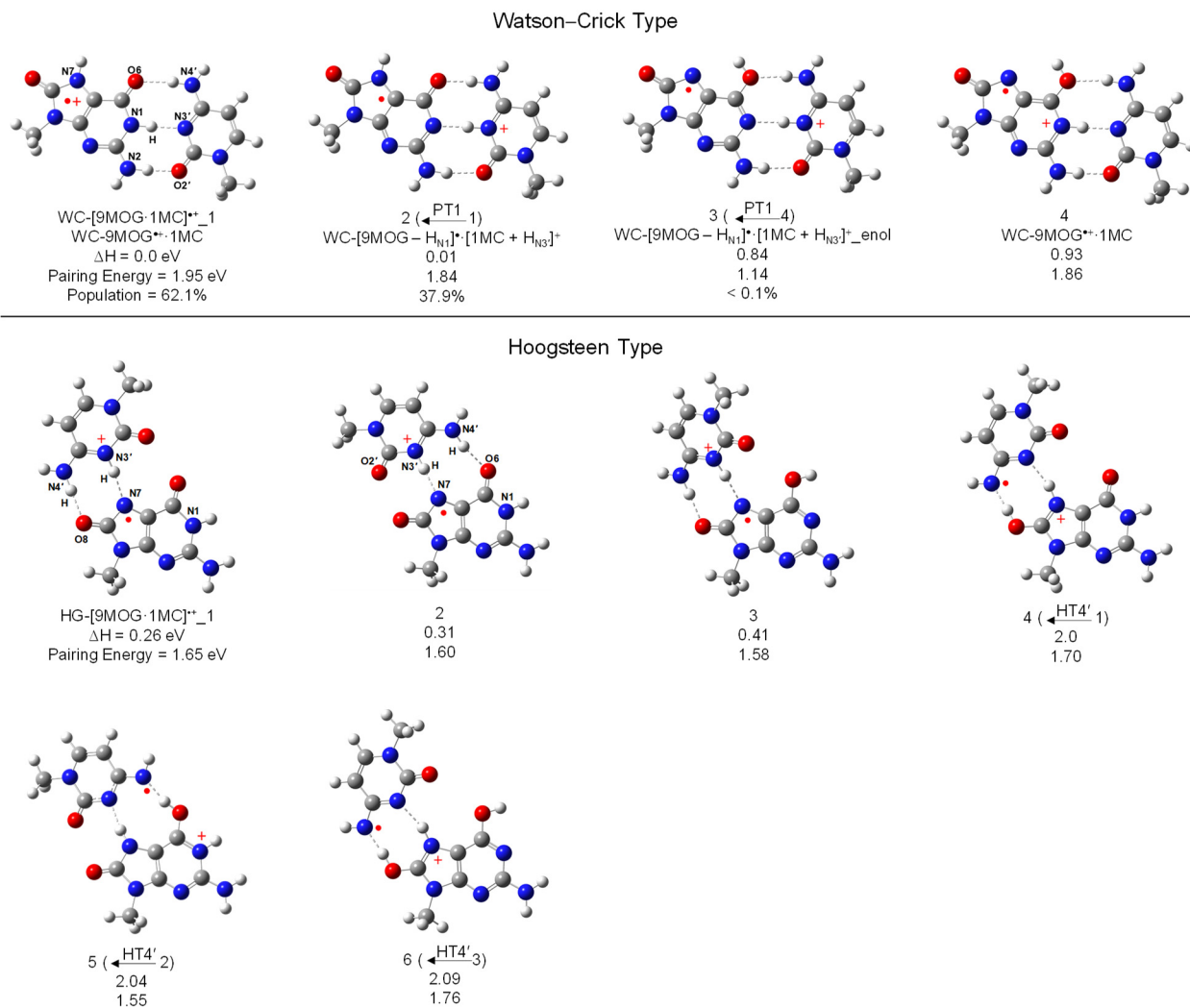
Supporting Information

Table of Contents

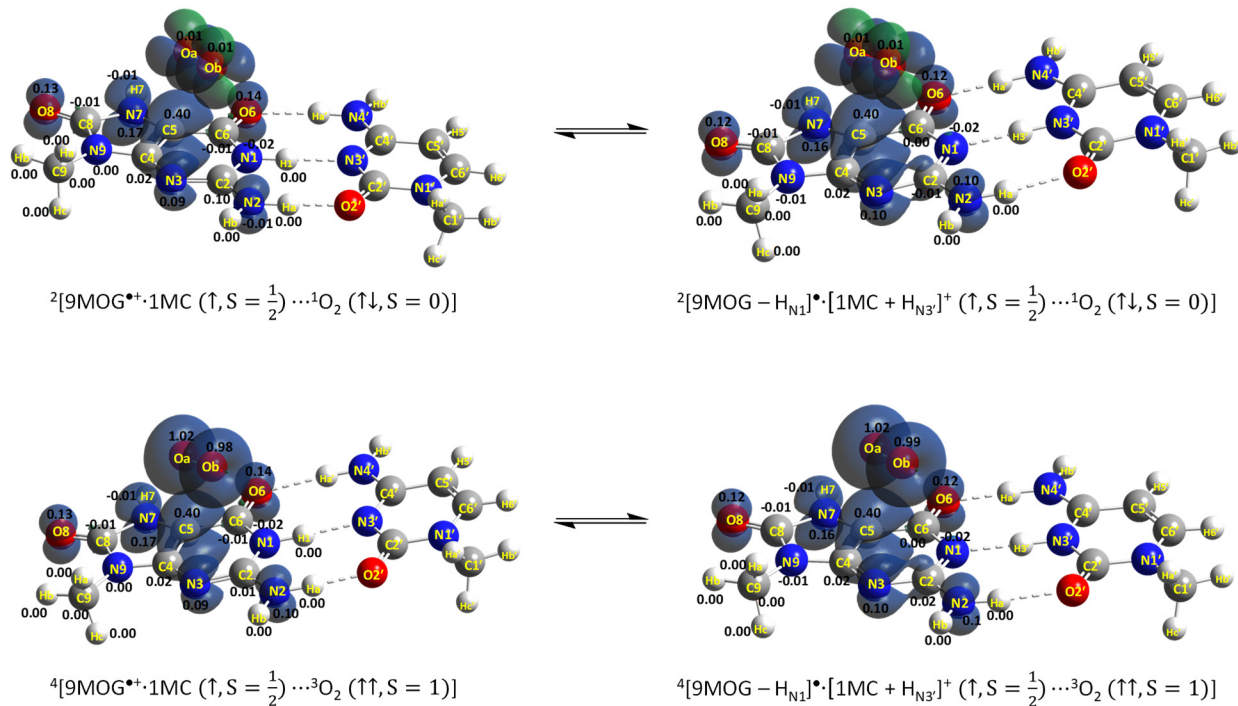
Scheme S1	$^1\text{O}_2$ -oxidation pathways of OG.....	S2
Scheme S2	Various conformers of $[\text{9MOG}\cdot\text{1MC}]^{\bullet+}$	S3
Scheme S3	Doublet and quartet states of the $^1\text{O}_2$ -adducts of $[\text{9MOG}\cdot\text{1MC}]^{\bullet+}$	S4
Scheme S4	$^1\text{O}_2$ -oxidation pathways of $\text{9MOG}^{\bullet+}$	S5
Scheme S5	$^1\text{O}_2$ -oxidation pathways of $[\text{9MOG} - \text{H}]^{\bullet}$	S6
Scheme S6	$^1\text{O}_2$ -oxidation pathways of $\text{9MOG}^{\bullet+}\cdot\text{1MC}$	S7
Scheme S7	$^1\text{O}_2$ -oxidation pathways of $[\text{9MOG} - \text{H}_{\text{N1}}]^{\bullet}\cdot[\text{1MC} + \text{H}_{\text{N3}}]^+$	S8
Table S1	Oxidation potentials and ionization potentials of DNA components.	S9
Table S2	Reaction energies for $^1\text{O}_2$ with $\text{9MOG}^{\bullet+}$ vs. $[\text{9MOG} - \text{H}]^{\bullet}$	S10
Table S3	Differences in AP-DFT, CASPT2 and NEVPT2 energy calculations	S11
	Cartesian coordinates for the structures in Scheme S2	S12
	Cartesian coordinates for the structures in Figure 2.....	S17
	Cartesian coordinates for the structures in Table S2.....	S20
	Cartesian coordinates for the structures in Table 1	S33



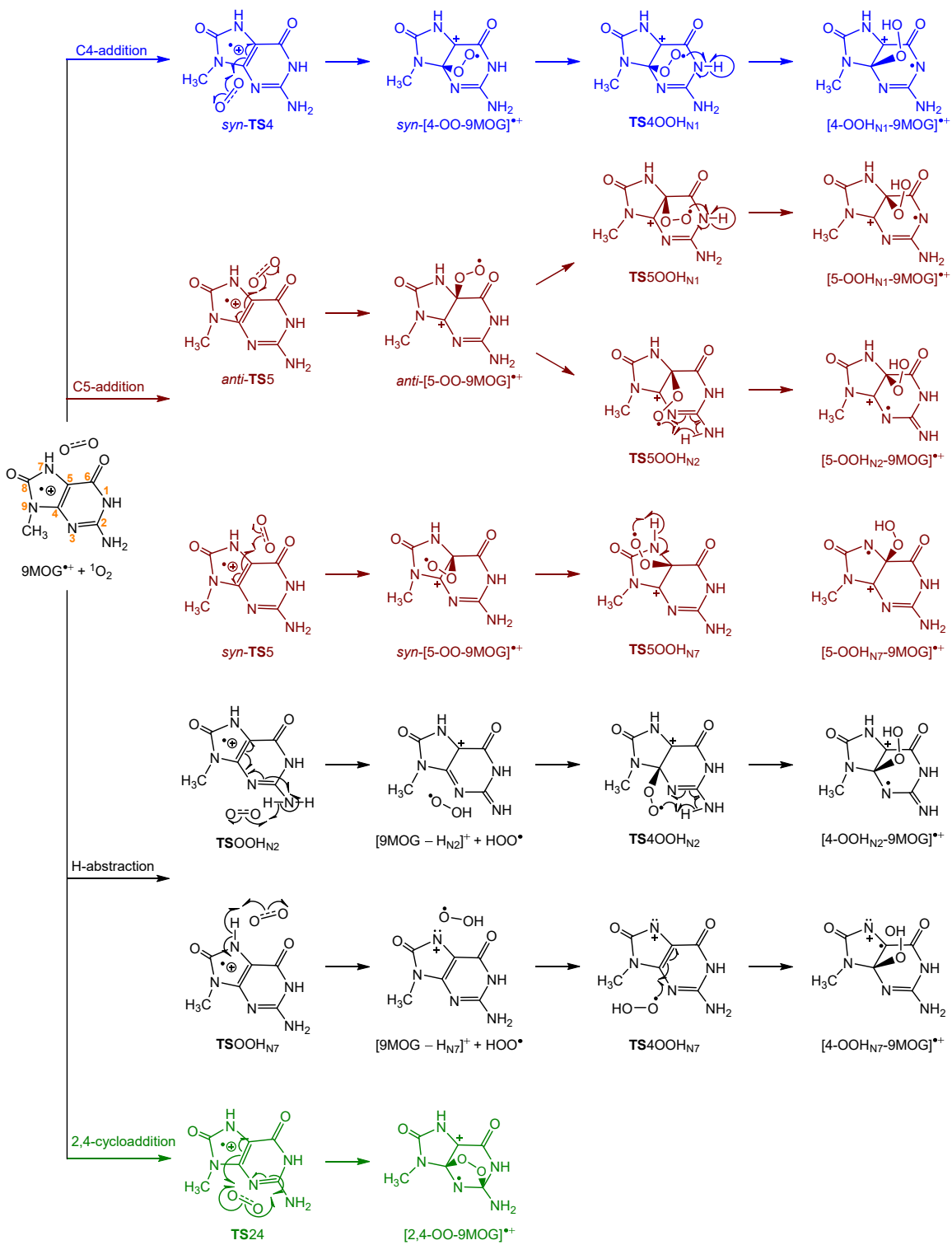
Scheme S1 The ${}^1\text{O}_2$ -oxidation pathways and products of OG reported in the literature.^[14a, 17b, 18a-1]



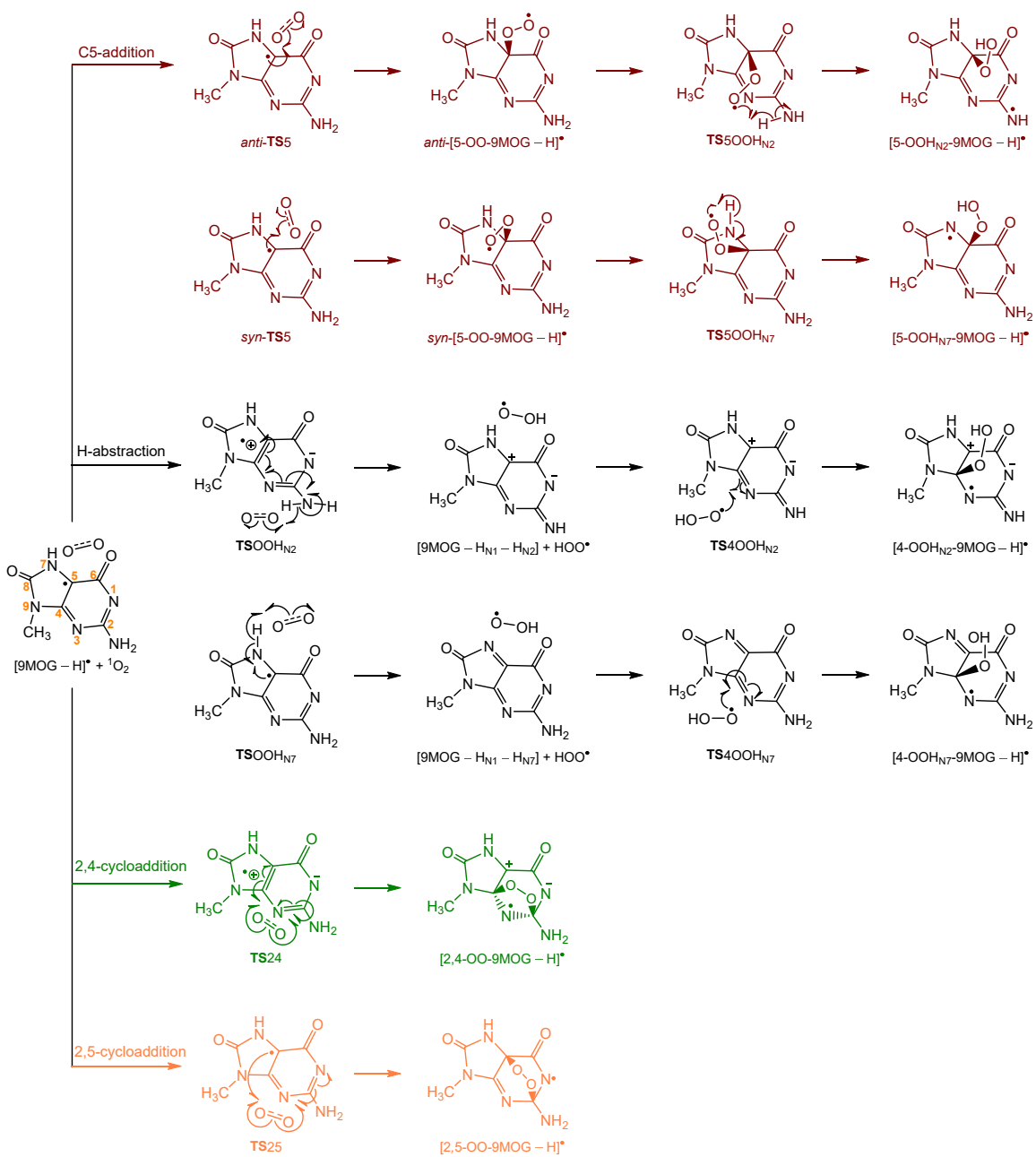
Scheme S2 Conformers of WC-[9MOG·1MC]^{•+} and HG-[9MOG·1MC]^{•+}. Dashed lines indicate H-bonds. Relative formation enthalpy (ΔH with respect to the global minimum), base-pairing energy and thermal populations were calculated at 298 K using the ω B97XD/6-311++G(d,p) level of theory, including thermal corrections.



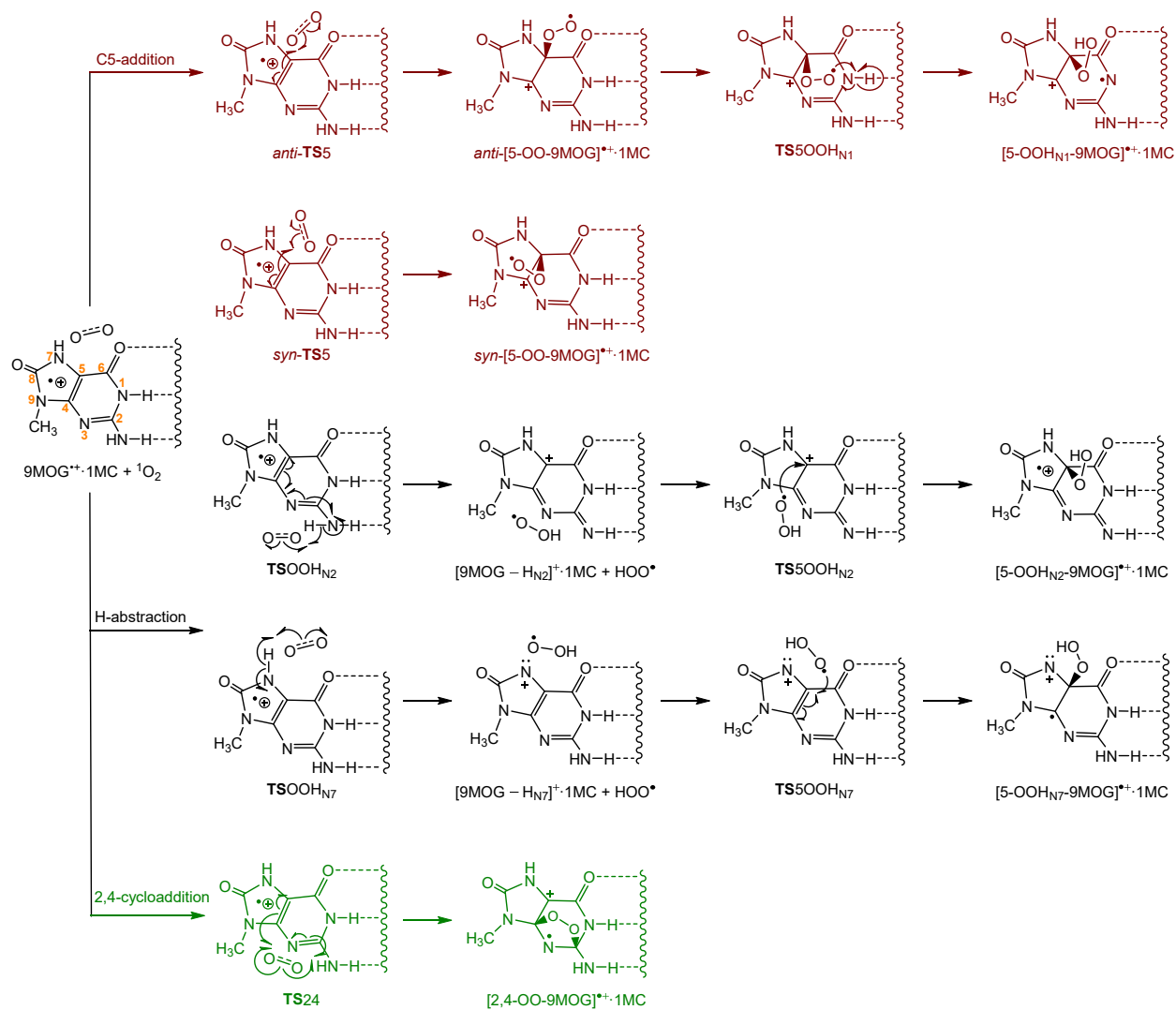
Scheme S3 Doublet and quartet electronic states of the 1O_2 reaction precursor complexes with $9MOG^{*+} \cdot 1MC$ and $[9MOG - H_{N1}]^{\bullet} \cdot [1MC + H_{N3}]^+$, with spin densities (numbers) calculated at $\omega B97XD/6-31+G(d,p)$.



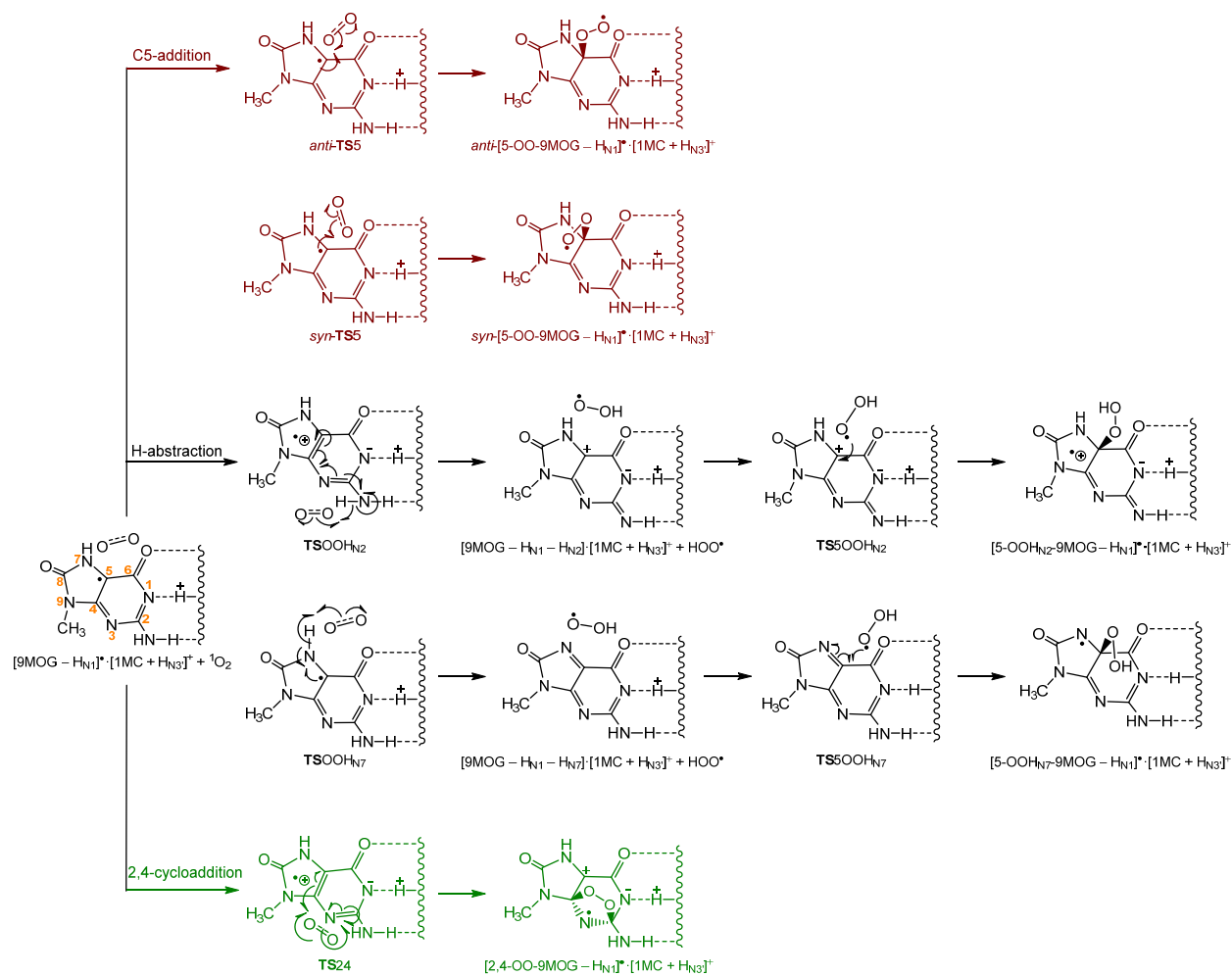
Scheme S4 Probable pathways and products for the ¹O₂ oxidation of 9MOG^{•+}.



Scheme S5 Probable pathways and products for the ¹O₂ oxidation of [9MOG - H]•.



Scheme S6 Probable pathways and products for the $^1\text{O}_2$ oxidation of 9MOG $^{*+}$ ·1MC, in which dashed lines represent base pair H-bonds.



Scheme S7 Probable pathways and products for the $^1\text{O}_2$ oxidation of $[\text{9MOG} - \text{H}_{\text{N}1}]^\bullet \cdot [\text{1MC} + \text{H}_{\text{N}3}]^\dagger$, in which dashed lines represent base pair H-bonds.

Table S1 Oxidation potentials (E° vs. NHE) and adiabatic ionization potentials (AIP) of DNA components.

species	E° (V)	species	AIP (eV)	
			gas phase	solution
8-oxoguanosine	0.74 ^[16]	8-oxoguanine	6.93 ^[15]	
guanosine	1.29 ^[4, 77]	guanine	7.68 ^[2]	4.42 ^[3]
adenosine	1.42 ^[4, 77]	adenine	8.26 ^[2b, 78]	4.81 ^[3]
deoxycytidine	1.6 ^[4, 77]	cytosine	8.66 ^[2b, 78]	4.91 ^[3]
thymidine	1.7 ^[4, 77]	thymine	8.82 ^[2b, 79]	5.05 ^[3]
		PO ₄ ³⁻	unstable	8.4 (vertical IP) ^[80]
		HPO ₄ ²⁻	unstable	8.9 ^[80]
		H ₂ PO ₄ ⁻	4.57 ^[81]	9.5 ^[80]
		deoxyribose		9.4-9.7 ^[80b, 82]

Table S2 Reaction energies (eV) for $^1\text{O}_2$ with 9MOG^{*+} versus $[9\text{MOG} - \text{H}]^*$ calculated at different levels of theory.

radical cations	AP- ω B97XD	CASPT2	NEVPT2	neutral radicals	AP- ω B97XD	CASPT2
$9\text{MOG}^{*+} + ^1\text{O}_2$	0.00	0.00	0.00	$[9\text{MOG} - \text{H}]^* + ^1\text{O}_2$	0.00	0.00
precursor	-0.39	-	-	precursor	-0.36	-
C4-addition						
<i>syn</i> -TS4	0.59	0.47	1.48			
<i>syn</i> -[4-OO-9MOG] $^{*+}$	0.57	0.43	1.74			
TS4OOH _{N1}	2.50	2.73	4.76			
[4-OOH _{N1} -9MOG] $^{*+}$	1.54	1.40	2.67			
C5-addition						
<i>syn/anti</i> -TS5	-0.71/-0.66	-0.94/-0.87	0.66/0.35	<i>syn/anti</i> -TS5	-0.97/-0.87	-1.21/-1.12
<i>syn/anti</i> -[5-OO-9MOG] $^{*+}$	-0.76/-0.76	-0.84/-0.84	-0.33/0.34	<i>syn/anti</i> -[5-OO-9MOG - H] *	-1.11/-1.08	-1.13/-1.17
TS5OOH _{N7}	1.01	1.16	2.14	TS5OOH _{N7}	0.67	0.35
[5-OOH _{N7} -9MOG] $^{*+}$	0.47	0.51	0.79	[5-OOH _{N7} -9MOG - H] *	0.10	0.15
TS5OOH _{N1}	1.05	1.03	1.66			
[5-OOH _{N1} -9MOG] $^{*+}$	0.29	0.02	1.84			
TS5OOH _{N2}	2.09	1.84	3.87	TS5OOH _{N2}	1.30	0.95
[5-OOH _{N2} -9MOG] $^{*+}$	0.62	0.60	1.11	[5-OOH _{N2} -9MOG - H] *	0.13	-0.09
H-abstraction						
TSOOH _{N2}	1.09	1.10	2.34			
$[9\text{MOG} - \text{H}_{\text{N}2}]^+ + \text{HOO}^\bullet$	1.17	0.93	1.35			
TS4OOH _{N2}	1.71	1.81	2.34			
[4-OOH _{N2} -9MOG] $^{*+}$	1.45	1.16	1.84			
TSOOH _{N7}	0.63	0.71	1.74	TSOOH _{N7}	-0.07	-0.36
$[9\text{MOG} - \text{H}_{\text{N}7}]^+ + \text{HOO}^\bullet$	0.23	0.25	0.38	$[9\text{MOG} - \text{H}_{\text{N}1} - \text{H}_{\text{N}7}] + \text{HOO}^\bullet$	-0.17	-0.36
TS4OOH _{N7}	1.63	1.73	2.57	TS4OOH _{N7}	0.96	0.63
[4-OOH _{N7} -9MOG] $^{*+}$	1.33	1.40	2.02	[4-OOH _{N7} -9MOG - H] *	0.53	0.29
2,4-cycloaddition						
TS24	1.77	2.16	3.56	TS24	1.78	1.76
[2,4-OO-9MOG] $^{*+}$	1.53	1.62	2.37	[2,4-OO-9MOG - H] *	1.41	1.16
2,5-cycloaddition						
				TS25	0.11	-0.05
				[2,5-OO-9MOG - H] *	0.11	0.02

Table S3 Differences in reaction energies calculated using AP- ω B97XD, CASPT2 and NEVPT2.

radical cations	$\Delta_{\text{CASPT2} - \text{AP-}\omega\text{B97XD}}$	$\Delta_{\text{NEVPT2} - \text{AP-}\omega\text{B97XD}}$	$\Delta_{\text{NEVPT2} - \text{CASPT2}}$	neutral radicals	$\Delta_{\text{CASPT2} - \text{AP-}\omega\text{B97XD}}$
9MOG ^{•+} + ¹ O ₂	0.00	0.00	0.00	[9MOG – H] [•] + ¹ O ₂	0.00
precursor	–	–	–	precursor	–
C4-addition					
<i>syn</i> -TS4	–0.12	0.89	1.01		
<i>syn</i> -[4-OO-9MOG] ^{•+}	–0.14	1.17	1.31		
TS4OOH _{N1}	0.23	2.26	2.03		
[4-OOH _{N1} -9MOG] ^{•+}	–0.14	1.13	1.27		
C5-addition					
<i>syn/anti</i> -TS5	–0.23/–0.21	1.37/1.01	1.60/1.22	<i>syn/anti</i> -TS5	–0.24/–0.25
<i>syn/anti</i> -[5-OO-9MOG] ^{•+}	–0.08/–0.08	0.43/1.10	0.51/1.18	<i>syn/anti</i> -[5-OO-9MG – H] [•]	–0.02/–0.09
TS5OOH _{N7}	0.15	1.13	0.98	TS5OOH _{N7}	–0.32
[5-OOH _{N7} -9MOG] ^{•+}	0.04	0.32	0.28	[5-OOH _{N7} -9MOG – H] [•]	0.05
TS5OOH _{N1}	–0.02	0.61	0.63		
[5-OOH _{N1} -9MOG] ^{•+}	–0.27	1.55	1.82		
TS5OOH _{N2}	–0.25	1.78	2.03	TS5OOH _{N2}	–0.35
[5-OOH _{N2} -9MOG] ^{•+}	–0.02	0.49	0.51	[5-OO-9MOG – H – H _{N2}] [•]	–0.22
H-abstraction					
TSOOH _{N2}	0.01	1.25	1.24		
[9MOG – H _{N2}] [•] + HOO [•]	–0.24	0.18	0.42		
TS4OOH _{N2}	0.10	0.63	0.53		
[4-OOH _{N2} -9MOG] ^{•+}	–0.29	0.39	0.68		
TSOOH _{N7}	0.08	1.11	1.03	TSOOH _{N7}	–0.29
[9MOG – H _{N7}] [•] + HOO [•]	0.02	0.15	0.13	[9MOG – H – H _{N7}] [•] + HOO [•]	–0.19
TS4OOH _{N7}	0.10	0.94	0.84	TS4OOH _{N7}	–0.33
[4-OOH _{N7} -9MOG] ^{•+}	0.07	0.69	0.62	[4-OOH _{N7} -9MOG – H] [•]	–0.24
2,4-cycloaddition					
TS24	0.39	1.79	1.40	TS24	–0.02
[2,4-OO-9MOG] ^{•+}	0.09	0.84	0.75	[2,4-OO-9MOG – H] [•]	–0.25
2,5-cycloaddition					
				TS25	–0.16
				[2,5-OO-9MOG – H] [•]	–0.09

**Cartesian coordinates for the structures
in Scheme S2, optimized at ω B97XD/
6-311++G(d,p).**

WC-[9MOG·1MC]⁺_1

C1 -1.098637 1.060814 -0.006876
 C2 -2.506033 0.747040 -0.005469
 H3 0.726245 0.075322 -0.004418
 C4 -0.817049 -1.359999 0.000812
 C5 -4.762427 0.710232 -0.003205
 N6 -0.319061 -0.085356 -0.004700
 N7 -3.599918 1.520206 -0.007566
 N8 -4.285257 -0.611181 -0.000101
 N9 -2.142834 -1.652950 0.005331
 C10 -2.930753 -0.614803 0.000973
 N11 0.035821 -2.354159 0.002124
 H12 -0.346664 -3.287419 0.006668
 H13 1.068482 -2.197929 -0.003005
 O14 -0.634264 2.185017 -0.009390
 C15 3.196809 -0.735333 -0.004523
 N16 2.461747 0.404006 -0.000694
 C17 3.057064 1.598334 0.006739
 C18 5.191209 0.567786 0.007340
 N19 4.585574 -0.645687 -0.001022
 H20 6.273977 0.560261 0.010181
 O21 2.681654 -1.857113 -0.011058
 N22 2.284974 2.687315 0.009409
 H23 1.272998 2.602640 0.002966
 H24 2.696410 3.604062 0.014132
 C25 4.479709 1.716573 0.011809
 H26 4.971958 2.677938 0.018577
 C27 5.351166 -1.892442 -0.007213
 H28 5.101001 -2.485153 0.872007
 H29 5.111921 -2.469718 -0.899712
 H30 6.412549 -1.650275 0.001478
 C31 -5.151207 -1.782326 0.017862
 H32 -4.868141 -2.455190 -0.790710
 H33 -5.062094 -2.296073 0.975080
 H34 -6.174060 -1.437994 -0.123401
 O35 -5.892286 1.084402 -0.004127
 H36 -3.631843 2.530483 -0.012211

Zero-point correction= 0.281156 (Hartree/Particle)
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 Thermal correction to Enthalpy= 0.302206
 Thermal correction to Gibbs Free Energy= 0.230519
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 Sum of electronic and thermal Enthalpies= -1090.820407
 Sum of electronic and thermal Free Energies= -1090.892094

WC-[9MOG·1MC]⁺_2

C1 -1.045000 0.936167 -0.014196
 C2 -2.471132 0.703716 -0.010013
 H3 1.442549 0.157944 -0.009807
 C4 -0.860356 -1.403582 -0.001526
 C5 -4.729135 0.768956 -0.002065

N6 -0.281306 -0.187590 -0.010842
 N7 -3.532834 1.524301 -0.012343
 N8 -4.315786 -0.569747 0.005005
 N9 -2.203183 -1.691857 0.008393
 C10 -2.956597 -0.633719 0.002612
 N11 -0.066094 -2.467238 -0.000917
 H12 -0.491182 -3.379726 0.006023
 H13 0.945669 -2.365260 -0.011226
 O14 -0.578758 2.082741 -0.019727
 C15 3.269380 -0.783722 -0.007946
 N16 2.483382 0.351263 -0.003088
 C17 2.953610 1.620420 0.009002
 C18 5.145180 0.691908 0.019771
 N19 4.638871 -0.567696 0.006943
 H20 6.225578 0.764341 0.028808
 O21 2.794636 -1.898390 -0.023552
 N22 2.094456 2.614752 0.008598
 H23 1.067261 2.448365 -0.003075
 H24 2.437419 3.561432 0.017349
 C25 4.365353 1.797625 0.021822
 H26 4.800641 2.785372 0.033301
 C27 5.499009 -1.755981 -0.007293
 H28 5.244018 -2.402252 0.831173
 H29 5.355154 -2.304784 -0.937505
 H30 6.535086 -1.434308 0.076606
 C31 -5.231335 -1.699323 0.029256
 H32 -4.983472 -2.386585 -0.779102
 H33 -5.161525 -2.217357 0.986097
 H34 -6.238815 -1.310246 -0.107152
 O35 -5.842926 1.197029 -0.001685
 H36 -3.518403 2.533919 -0.020571

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WC-[9MOG·1MC]⁺_3

C1 -1.169640 0.863414 -0.151462
 C2 -2.556289 0.695449 -0.089502
 H3 1.465224 0.186113 -0.084300
 C4 -0.903704 -1.408782 0.007803
 C5 -4.707087 0.810122 -0.012723
 N6 -0.340960 -0.159259 -0.099149
 N7 -3.535761 1.581678 -0.119487
 N8 -4.341018 -0.581413 0.082157
 N9 -2.217002 -1.705002 0.085858
 C10 -3.006355 -0.657691 0.035925
 N11 -0.062069 -2.440371 0.040896
 H12 -0.457488 -3.363984 0.101856
 H13 0.938611 -2.318422 -0.064856
 O14 -0.643152 2.093154 -0.261146
 C15 3.275308 -0.788736 -0.089653

N16 2.500553 0.359771 -0.031455
 C17 2.991119 1.610112 0.112707
 C18 5.164642 0.649753 0.150016
 N19 4.645812 -0.592085 0.002295
 H20 6.244015 0.705621 0.217757
 O21 2.789193 -1.887624 -0.210571
 N22 2.151027 2.627469 0.156937
 H23 1.145850 2.500205 0.044915
 H24 2.507886 3.563170 0.261277
 C25 4.396770 1.765124 0.211287
 H26 4.842019 2.741412 0.328403
 C27 5.490123 -1.792017 -0.064926
 H28 5.212982 -2.479222 0.733095
 H29 5.349689 -2.285196 -1.025954
 H30 6.529192 -1.490651 0.049655
 C31 -5.288065 -1.672274 0.214025
 H32 -5.125202 -2.405201 -0.576606
 H33 -5.178014 -2.153306 1.186778
 H34 -6.286845 -1.247800 0.125494
 O35 -5.839211 1.198195 0.001124
 H36 -1.367570 2.735100 -0.300115

Zero-point correction= 0.281696 (Hartree/Particle)
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 Thermal correction to Gibbs Free Energy= 0.231186
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 Sum of electronic and thermal Energies= -1090.790315
 Sum of electronic and thermal Enthalpies= -1090.789371
 Sum of electronic and thermal Free Energies= -1090.860894

WC-[9MOG·1MC]⁺_4

C1 -1.188177 0.958209 -0.121843
 C2 -2.556437 0.731803 -0.076519
 H3 0.682745 0.074776 -0.065685
 C4 -0.864066 -1.394280 0.030055
 C5 -4.711666 0.785946 -0.027201
 N6 -0.360922 -0.101397 -0.064907
 N7 -3.558757 1.591587 -0.112861
 N8 -4.305671 -0.600327 0.061912
 N9 -2.173411 -1.679690 0.085992
 C10 -2.975861 -0.642651 0.033094
 N11 0.012104 -2.371149 0.065964
 H12 -0.355589 -3.307830 0.130951
 H13 1.034492 -2.204884 -0.017583
 O14 -0.643410 2.154012 -0.215493
 C15 3.172265 -0.729078 -0.067957
 N16 2.458057 0.426856 -0.001077
 C17 3.089035 1.595928 0.111113
 C18 5.196804 0.518571 0.092661
 N19 4.562901 -0.672257 -0.024767
 H20 6.278569 0.483799 0.123721
 O21 2.636772 -1.833666 -0.165321
 N22 2.349996 2.710718 0.173985
 H23 1.346954 2.657637 0.094842
 H24 2.785083 3.613682 0.244086
 C25 4.510362 1.680720 0.166606

H26 5.021652 2.627372 0.260511
 C27 5.298689 -1.935185 -0.106977
 H28 4.991933 -2.594887 0.703589
 H29 5.089174 -2.425261 -1.057207
 H30 6.363501 -1.723590 -0.027367
 C31 -5.228095 -1.718063 0.172806
 H32 -5.026861 -2.443023 -0.615703
 H33 -5.123979 -2.194992 1.147769
 H34 -6.235243 -1.319322 0.063589
 O35 -5.850033 1.141460 -0.025803
 H36 -1.346269 2.820167 -0.257259

Zero-point correction= 0.280653 (Hartree/Particle)
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 Thermal correction to Enthalpy= 0.301774
 Thermal correction to Gibbs Free Energy= 0.229730
 Sum of electronic and zero-point Energies= -1090.807366
 Sum of electronic and thermal Energies= -1090.787190
 Sum of electronic and thermal Enthalpies= -1090.786245
 Sum of electronic and thermal Free Energies= -1090.858289

HG-[9MOG·1MC]⁺_1

C1 -1.705378 -1.638718 -0.495603
 C2 -1.600807 -0.225454 -0.198860
 H3 -3.187531 -3.060080 -0.544585
 C4 -4.116969 -1.287166 -0.033239
 C5 -1.021743 1.837279 0.085952
 N6 -3.053492 -2.075498 -0.353664
 N7 -0.540720 0.571514 -0.197835
 N8 -2.415954 1.780344 0.280675
 N9 -4.023269 0.019835 0.197751
 C10 -2.794657 0.498964 0.104591
 N11 -5.324323 -1.851802 0.052438
 H12 -6.102697 -1.258592 0.290000
 H13 -5.485890 -2.832791 -0.096743
 O14 -0.844554 -2.405307 -0.835072
 C15 2.804439 -0.963420 0.395716
 N16 2.268485 0.269931 0.033639
 C17 2.980623 1.346230 -0.356924
 C18 4.926579 -0.010587 -0.186964
 N19 4.191232 -1.061484 0.239968
 H20 5.992624 -0.183516 -0.269268
 O21 2.131830 -1.866444 0.806390
 N22 2.350844 2.482273 -0.598790
 H23 1.356626 2.622762 -0.372463
 H24 2.885428 3.285018 -0.886615
 C25 4.386354 1.196267 -0.488348
 H26 5.006513 2.019585 -0.808423
 C27 4.793673 -2.351320 0.586800
 H28 4.602582 -2.575999 1.635652
 H29 4.356861 -3.137384 -0.027997
 H30 5.865690 -2.292863 0.408794
 C31 -3.268910 2.912115 0.598838
 H32 -4.034952 3.027738 -0.168058
 H33 -3.742592 2.761951 1.569197
 H34 -2.638624 3.799076 0.629000
 O35 -0.358236 2.858154 0.151594

H36 1.224793 0.302937 0.007180

Zero-point correction= 0.281162 (Hartree/Particle)
Thermal correction to Energy= 0.301650
Thermal correction to Enthalpy= 0.302594
Thermal correction to Gibbs Free Energy= 0.230153
Sum of electronic and zero-point Energies= -1090.832194
Sum of electronic and thermal Energies= -1090.811706
Sum of electronic and thermal Enthalpies= -1090.810762
Sum of electronic and thermal Free Energies= -1090.883203

HG-[9MOG·1MC]⁺_2

C1 1.893739 -1.577594 0.119664
C2 1.637706 -0.184423 -0.084376
H3 3.487944 -2.794526 0.524579
C4 4.232531 -0.862581 0.389811
C5 0.810524 1.775644 -0.522525
N6 3.252994 -1.822340 0.372545
N7 0.489862 0.427212 -0.337240
N8 2.224602 1.930259 -0.332402
N9 4.009387 0.422837 0.165780
C10 2.737994 0.725825 -0.068344
N11 5.484594 -1.256269 0.643479
H12 6.201853 -0.549329 0.657846
H13 5.736615 -2.209381 0.839308
O14 1.092179 -2.497739 0.081722
C15 -3.044844 0.611662 0.513911
N16 -2.182229 -0.379318 0.050088
C17 -2.561965 -1.566320 -0.459300
C18 -4.811501 -0.842492 -0.203872
N19 -4.403836 0.325265 0.339020
H20 -5.883035 -0.972734 -0.293423
O21 -2.654831 1.624725 1.020355
N22 -1.632737 -2.445351 -0.797972
H23 -0.648003 -2.337871 -0.534127
H24 -1.917136 -3.336750 -1.168678
C25 -3.951302 -1.811626 -0.607384
H26 -4.313705 -2.741056 -1.019185
C27 -5.345484 1.352680 0.792016
H28 -5.210837 1.528196 1.858787
H29 -5.159482 2.282840 0.256288
H30 -6.358727 1.007097 0.596551
C31 2.935109 3.191881 -0.437141
H32 3.408426 3.434433 0.514575
H33 3.692870 3.131387 -1.218640
H34 2.202057 3.955757 -0.690696
O35 0.068197 2.673491 -0.807395
H36 -1.176702 -0.093888 0.001512

Zero-point correction= 0.280995 (Hartree/Particle)
Thermal correction to Energy= 0.301549
Thermal correction to Enthalpy= 0.302493
Thermal correction to Gibbs Free Energy= 0.229981
Sum of electronic and zero-point Energies= -1090.830520
Sum of electronic and thermal Energies= -1090.809966
Sum of electronic and thermal Enthalpies= -1090.809022
Sum of electronic and thermal Free Energies= -1090.881535

HG-[9MOG·1MC]⁺_3

C1 -1.851453 -1.634800 -0.363981
C2 -1.648376 -0.240655 -0.165520
H3 -1.118743 -3.310599 -0.729503
C4 -4.095877 -1.320194 -0.012729
C5 -1.060500 1.828579 0.047639
N6 -3.053659 -2.147557 -0.278984
N7 -0.576839 0.543277 -0.176619
N8 -2.451668 1.796967 0.213045
N9 -4.055184 0.021511 0.168831
C10 -2.846427 0.508322 0.084384
N11 -5.293481 -1.896094 0.074331
H12 -6.103333 -1.330759 0.268457
H13 -5.381279 -2.890288 -0.053943
O14 -0.818551 -2.396490 -0.644774
C15 2.808604 -0.979950 0.283632
N16 2.263566 0.272341 0.012008
C17 2.972643 1.386484 -0.269058
C18 4.936991 0.053776 -0.104962
N19 4.202354 -1.039883 0.202401
H20 6.009152 -0.094500 -0.144463
O21 2.134449 -1.931982 0.564428
N22 2.337763 2.526711 -0.461217
H23 1.324890 2.637082 -0.298850
H24 2.873593 3.353792 -0.666878
C25 4.386438 1.268490 -0.343932
H26 5.002847 2.124049 -0.574199
C27 4.815421 -2.342345 0.475994
H28 4.564704 -2.662285 1.486816
H29 4.442006 -3.081253 -0.232047
H30 5.894542 -2.245406 0.374631
C31 -3.299040 2.947453 0.472559
H32 -4.055128 3.034812 -0.307836
H33 -3.786351 2.840530 1.442001
H34 -2.664135 3.831567 0.473879
O35 -0.383768 2.841736 0.090573
H36 1.219700 0.295284 -0.020601

Zero-point correction= 0.281745 (Hartree/Particle)
Thermal correction to Energy= 0.301928
Thermal correction to Enthalpy= 0.302873
Thermal correction to Gibbs Free Energy= 0.230834
Sum of electronic and zero-point Energies= -1090.826506
Sum of electronic and thermal Energies= -1090.806322
Sum of electronic and thermal Enthalpies= -1090.805378
Sum of electronic and thermal Free Energies= -1090.877417

HG-[9MOG·1MC]⁺_4

C1 -1.861533 -1.717584 -0.385588
C2 -1.679364 -0.327064 -0.105397
H3 -3.458802 -2.995058 -0.495534
C4 -4.260099 -1.138411 -0.054790
C5 -0.940375 1.729895 0.118842
N6 -3.247311 -2.025862 -0.298224
N7 -0.544714 0.478887 -0.095152
N8 -2.283064 1.777411 0.240582
N9 -4.058261 0.145534 0.146393

C10 -2.762647 0.483413 0.100795
 N11 -5.519671 -1.615069 -0.045740
 H12 -6.256051 -0.972602 0.192799
 H13 -5.725604 -2.598087 -0.057773
 O14 -1.049998 -2.561955 -0.670621
 C15 2.868757 -0.938295 0.389616
 N16 2.294921 0.262904 0.072345
 C17 3.033906 1.289644 -0.340152
 C18 5.019045 -0.010345 -0.267407
 N19 4.287119 -1.041638 0.161754
 H20 6.081178 -0.182607 -0.394743
 O21 2.276876 -1.887093 0.831764
 N22 2.351446 2.442725 -0.548589
 H23 0.748449 2.638035 -0.071708
 H24 2.958686 3.190275 -0.884571
 C25 4.438915 1.204545 -0.530756
 H26 5.029953 2.044816 -0.865212
 C27 4.881456 -2.343869 0.456143
 H28 4.721395 -2.579580 1.508372
 H29 4.383249 -3.106621 -0.142393
 H30 5.945153 -2.312223 0.228498
 C31 -3.094482 2.966409 0.466795
 H32 -3.867355 3.020611 -0.298422
 H33 -3.558847 2.909581 1.450731
 H34 -2.449561 3.840459 0.410383
 O35 -0.205516 2.791669 0.210333
 H36 0.452534 0.197787 -0.074410

Zero-point correction= 0.278233 (Hartree/Particle)
 Thermal correction to Energy= 0.298894
 Thermal correction to Enthalpy= 0.299838
 Thermal correction to Gibbs Free Energy= 0.226426
 Sum of electronic and zero-point Energies= -1090.768434
 Sum of electronic and thermal Energies= -1090.747773
 Sum of electronic and thermal Enthalpies= -1090.746829
 Sum of electronic and thermal Free Energies= -1090.820241

HG-[9MOG·1MC]⁺₅

C1 1.776691 -1.499198 0.071801
 C2 1.584321 -0.165356 -0.113406
 H3 3.210469 -2.873268 0.518844
 C4 4.115063 -1.007622 0.439506
 C5 0.918925 1.939662 -0.570028
 N6 3.070625 -1.882250 0.374614
 N7 0.504079 0.626072 -0.456537
 N8 2.330280 1.915892 -0.345254
 N9 3.969759 0.282456 0.208077
 C10 2.726814 0.666745 -0.062148
 N11 5.330807 -1.489156 0.739302
 H12 6.089082 -0.830095 0.800645
 H13 5.504068 -2.451009 0.971572
 O14 0.940894 -2.502502 0.023029
 C15 -3.032659 0.551111 0.594928
 N16 -2.147491 -0.372579 0.105346
 C17 -2.572127 -1.471652 -0.507347
 C18 -4.841144 -0.822292 -0.271878
 N19 -4.424007 0.282516 0.355474

H20 -5.910905 -0.938363 -0.398283
 O21 -2.721701 1.547891 1.193151
 N22 -1.590306 -2.328302 -0.890910
 H23 0.024569 -2.288755 -0.321378
 H24 -1.970373 -3.134292 -1.388597
 C25 -3.946877 -1.754107 -0.729658
 H26 -4.282237 -2.652037 -1.227996
 C27 -5.357700 1.293144 0.847123
 H28 -5.226127 1.409401 1.922798
 H29 -5.132610 2.248720 0.372872
 H30 -6.375616 0.984197 0.617296
 C31 3.163740 3.103927 -0.398511
 H32 3.637234 3.272240 0.568877
 H33 3.928109 2.992460 -1.167786
 H34 2.511297 3.940966 -0.642047
 O35 0.274643 2.916874 -0.815086
 H36 -0.474151 0.373019 -0.268659

Zero-point correction= 0.278381 (Hartree/Particle)
 Thermal correction to Energy= 0.298929
 Thermal correction to Enthalpy= 0.299873
 Thermal correction to Gibbs Free Energy= 0.227346
 Sum of electronic and zero-point Energies= -1090.767003
 Sum of electronic and thermal Energies= -1090.746456
 Sum of electronic and thermal Enthalpies= -1090.745512
 Sum of electronic and thermal Free Energies= -1090.818038

HG-[9MOG·1MC]⁺₆

C1 -2.007541 -1.691518 -0.198888
 C2 -1.720247 -0.334441 -0.061717
 H3 -1.420505 -3.449792 -0.414307
 C4 -4.245491 -1.181213 -0.044288
 C5 -0.981547 1.733010 0.075297
 N6 -3.260648 -2.095824 -0.181244
 N7 -0.577647 0.469856 -0.047924
 N8 -2.325920 1.799294 0.134896
 N9 -4.083961 0.147846 0.071671
 C10 -2.816597 0.501129 0.055292
 N11 -5.503878 -1.654874 -0.027318
 H12 -6.273561 -1.018087 0.075703
 H13 -5.665336 -2.642446 -0.110565
 O14 -1.029824 -2.569915 -0.350123
 C15 2.871097 -0.971933 0.211806
 N16 2.298770 0.258609 0.036443
 C17 3.046538 1.333277 -0.202154
 C18 5.045316 0.054694 -0.148781
 N19 4.303657 -1.028784 0.099747
 H20 6.117001 -0.090310 -0.215217
 O21 2.261793 -1.983457 0.446986
 N22 2.361743 2.497110 -0.323059
 H23 0.726671 2.639499 -0.036334
 H24 2.978303 3.285156 -0.521649
 C25 4.462026 1.284679 -0.310376
 H26 5.057555 2.164470 -0.506752
 C27 4.903193 -2.349358 0.280660
 H28 4.655478 -2.722785 1.274403
 H29 4.485173 -3.036406 -0.455115

H30 5.981861 -2.271312 0.160182
C31 -3.123304 3.009437 0.283379
H32 -4.086532 2.832899 -0.191477
H33 -3.273403 3.234052 1.339609
H34 -2.610414 3.836849 -0.203057
O35 -0.254025 2.798970 0.134882
H36 0.418692 0.194209 -0.033248

Zero-point correction= 0.278435 (Hartree/Particle)
Thermal correction to Energy= 0.298841
Thermal correction to Enthalpy= 0.299785
Thermal correction to Gibbs Free Energy= 0.226970
Sum of electronic and zero-point Energies= -1090.765001
Sum of electronic and thermal Energies= -1090.744596
Sum of electronic and thermal Enthalpies= -1090.743652
Sum of electronic and thermal Free Energies= -1090.816467

**Cartesian coordinates for the structures
in Figure 2, optimized at ω B97XD/
6-311++G(d,p).**

9MOG⁺·1MC

C1 -1.098637 1.060814 -0.006876
 C2 -2.506033 0.747040 -0.005469
 H3 0.726245 0.075322 -0.004418
 C4 -0.817049 -1.359999 0.000812
 C5 -4.762427 0.710232 -0.003205
 N6 -0.319061 -0.085356 -0.004700
 N7 -3.599918 1.520206 -0.007566
 N8 -4.285257 -0.611181 -0.000101
 N9 -2.142834 -1.652950 0.005331
 C10 -2.930753 -0.614803 0.000973
 N11 0.035821 -2.354159 0.002124
 H12 -0.346664 -3.287419 0.006668
 H13 1.068482 -2.197929 -0.003005
 O14 -0.634264 2.185017 -0.009390
 C15 3.196809 -0.735333 -0.004523
 N16 2.461747 0.404006 -0.000694
 C17 3.057064 1.598334 0.006739
 C18 5.191209 0.567786 0.007340
 N19 4.585574 -0.645687 -0.001022
 H20 6.273977 0.560261 0.010181
 O21 2.681654 -1.857113 -0.011058
 N22 2.284974 2.687315 0.009409
 H23 1.272998 2.602640 0.002966
 H24 2.696410 3.604062 0.014132
 C25 4.479709 1.716573 0.011809
 H26 4.971958 2.677938 0.018577
 C27 5.351166 -1.892442 -0.007213
 H28 5.101001 -2.485153 0.872007
 H29 5.111921 -2.469718 -0.899712
 H30 6.412549 -1.650275 0.001478
 C31 -5.151207 -1.782326 0.017862
 H32 -4.868141 -2.455190 -0.790710
 H33 -5.062094 -2.296073 0.975080
 H34 -6.174060 -1.437994 -0.123401
 O35 -5.892286 1.084402 -0.004127
 H36 -3.631843 2.530483 -0.012211

Zero-point correction= 0.281156 (Hartree/Particle)
 Thermal correction to Energy= 0.301262
 Thermal correction to Enthalpy= 0.302206
 Thermal correction to Gibbs Free Energy= 0.230519
 Sum of electronic and zero-point Energies= -1090.841457
 Sum of electronic and thermal Energies= -1090.821351
 Sum of electronic and thermal Enthalpies= -1090.820407
 Sum of electronic and thermal Free Energies= -1090.892094

TS-PT

C1 -1.017369 0.996674 -0.099499
 C2 -2.431080 0.713841 -0.074105
 H3 1.074449 0.116099 -0.039809
 C4 -0.760663 -1.365658 0.035065
 C5 -4.687642 0.721440 -0.031569

N6 -0.214806 -0.118222 -0.042644
 N7 -3.511657 1.506951 -0.107624
 N8 -4.235744 -0.604653 0.052751
 N9 -2.094158 -1.664077 0.087933
 C10 -2.878706 -0.630045 0.030356
 N11 0.046331 -2.405456 0.065637
 H12 -0.378755 -3.317455 0.118741
 H13 1.066033 -2.297310 -0.019046
 O14 -0.589746 2.145648 -0.161857
 C15 3.155537 -0.753729 -0.076028
 N16 2.360948 0.362358 -0.016353
 C17 2.895536 1.596404 0.090464
 C18 5.076299 0.648655 0.102251
 N19 4.532887 -0.587204 -0.017908
 H20 6.157197 0.693347 0.146019
 O21 2.696801 -1.883199 -0.175986
 N22 2.093906 2.647750 0.128374
 H23 1.078027 2.546168 0.024238
 H24 2.489818 3.569635 0.199177
 C25 4.310480 1.758436 0.161760
 H26 4.754639 2.738286 0.254406
 C27 5.359265 -1.794963 -0.088618
 H28 5.091114 -2.473696 0.719794
 H29 5.197879 -2.298912 -1.040916
 H30 6.404289 -1.505300 0.003963
 C31 -5.120152 -1.755700 0.156662
 H32 -4.884169 -2.469666 -0.631836
 H33 -5.001986 -2.230391 1.130852
 H34 -6.141584 -1.397509 0.041366
 O35 -5.811538 1.117268 -0.039768
 H36 -3.524061 2.514697 -0.177672

Zero-point correction= 0.277297 (Hartree/Particle)
 Thermal correction to Energy= 0.296878
 Thermal correction to Enthalpy= 0.297822
 Thermal correction to Gibbs Free Energy= 0.227497
 Sum of electronic and zero-point Energies= -1090.838172
 Sum of electronic and thermal Energies= -1090.818590
 Sum of electronic and thermal Enthalpies= -1090.817646
 Sum of electronic and thermal Free Energies= -1090.887971

[9MOG - H_{N1}]⁺·[1MC + H_{N3}]⁺

C1 -1.045000 0.936167 -0.014196
 C2 -2.471132 0.703716 -0.010013
 H3 1.442549 0.157944 -0.009807
 C4 -0.860356 -1.403582 -0.001526
 C5 -4.729135 0.768956 -0.002065
 N6 -0.281306 -0.187590 -0.010842
 N7 -3.532834 1.524301 -0.012343
 N8 -4.315786 -0.569747 0.005005
 N9 -2.203183 -1.691857 0.008393
 C10 -2.956597 -0.633719 0.002612
 N11 -0.066094 -2.467238 -0.000917
 H12 -0.491182 -3.379726 0.006023
 H13 0.945669 -2.365260 -0.011226
 O14 -0.578758 2.082741 -0.019727
 C15 3.269380 -0.783722 -0.007946

N16 2.483382 0.351263 -0.003088
 C17 2.953610 1.620420 0.009002
 C18 5.145180 0.691908 0.019771
 N19 4.638871 -0.567696 0.006943
 H20 6.225578 0.764341 0.028808
 O21 2.794636 -1.898390 -0.023552
 N22 2.094456 2.614752 0.008598
 H23 1.067261 2.448365 -0.003075
 H24 2.437419 3.561432 0.017349
 C25 4.365353 1.797625 0.021822
 H26 4.800641 2.785372 0.033301
 C27 5.499009 -1.755981 -0.007293
 H28 5.244018 -2.402252 0.831173
 H29 5.355154 -2.304784 -0.937505
 H30 6.535086 -1.434308 0.076606
 C31 -5.231335 -1.699323 0.029256
 H32 -4.983472 -2.386585 -0.779102
 H33 -5.161525 -2.217357 0.986097
 H34 -6.238815 -1.310246 -0.107152
 O35 -5.842926 1.197029 -0.001685
 H36 -3.518403 2.533919 -0.020571

Zero-point correction= 0.281414 (Hartree/Particle)
 Thermal correction to Energy= 0.301508
 Thermal correction to Enthalpy= 0.302453
 Thermal correction to Gibbs Free Energy= 0.230682
 Sum of electronic and zero-point Energies= -1090.840973
 Sum of electronic and thermal Energies= -1090.820879
 Sum of electronic and thermal Enthalpies= -1090.819935
 Sum of electronic and thermal Free Energies= -1090.891705

9MOG⁺

C1 1.261357 1.483533 0.000736
 C2 -0.057794 0.899485 0.001156
 H3 3.199490 0.810088 -0.000111
 C4 1.993296 -0.873416 -0.000485
 C5 -2.262870 0.436519 -0.000792
 N6 2.246226 0.466654 -0.000134
 N7 -1.275271 1.452014 0.001061
 N8 -1.538239 -0.775901 -0.002779
 N9 0.759287 -1.396544 0.000514
 C10 -0.217381 -0.519264 0.000353
 N11 3.015074 -1.717509 -0.001510
 H12 2.810123 -2.705534 -0.001119
 H13 3.978410 -1.423233 -0.002503
 O14 1.539890 2.651554 0.001102
 C15 -2.171771 -2.090312 0.003496
 H16 -1.996783 -2.581349 0.960530
 H17 -3.239346 -1.940277 -0.145675
 H18 -1.761963 -2.692477 -0.806228
 O19 -3.441203 0.582572 -0.002657
 H20 -1.497986 2.439504 0.000701

Zero-point correction= 0.151234 (Hartree/Particle)
 Thermal correction to Energy= 0.162256
 Thermal correction to Enthalpy= 0.163200
 Thermal correction to Gibbs Free Energy= 0.113871
 Sum of electronic and zero-point Energies= -656.675467

Sum of electronic and thermal Energies= -656.664444
 Sum of electronic and thermal Enthalpies= -656.663500
 Sum of electronic and thermal Free Energies= -656.712830

1MC

C1 -1.536977 -0.033495 0.002257
 C2 -1.076252 1.322992 0.001068
 C3 0.265977 1.493961 -0.000483
 H4 -1.751207 2.166725 0.008661
 H5 0.723004 2.476723 -0.000478
 N6 -0.733676 -1.069031 -0.001581
 C7 0.620814 -0.898799 0.000283
 O8 1.430823 -1.802102 -0.000464
 N9 1.110749 0.440485 -0.000410
 C10 2.555970 0.612484 -0.001696
 H11 2.989249 0.139041 0.879877
 H12 2.987771 0.140913 -0.885030
 H13 2.786087 1.678197 -0.000708
 N14 -2.870707 -0.282567 0.028971
 H15 -3.538650 0.449909 -0.126031
 H16 -3.164592 -1.239747 -0.070019

Zero-point correction= 0.127303 (Hartree/Particle)
 Thermal correction to Energy= 0.135617
 Thermal correction to Enthalpy= 0.136561
 Thermal correction to Gibbs Free Energy= 0.094444
 Sum of electronic and zero-point Energies= -434.094496
 Sum of electronic and thermal Energies= -434.086182
 Sum of electronic and thermal Enthalpies= -434.085238
 Sum of electronic and thermal Free Energies= -434.127356

[9MOG - H][•]

C1 1.338047 1.439829 0.001018
 C2 -0.004850 0.870869 0.000984
 C3 2.039509 -0.779548 -0.000425
 C4 -2.224101 0.433668 -0.001156
 N5 2.337289 0.500571 0.000062
 N6 -1.232684 1.429075 0.000110
 N7 -1.527833 -0.776258 -0.002859
 N8 0.790742 -1.397710 0.000821
 C9 -0.177332 -0.535734 0.000542
 N10 3.055884 -1.662560 -0.002201
 H11 2.860867 -2.647331 -0.001796
 H12 3.999215 -1.316372 -0.002972
 O13 1.506547 2.649790 0.001763
 C14 -2.163241 -2.077726 0.003834
 H15 -1.974017 -2.587647 0.949755
 H16 -3.233767 -1.924432 -0.123408
 H17 -1.773406 -2.681765 -0.815984
 O18 -3.413637 0.597730 -0.002501
 H19 -1.434151 2.417411 -0.000014

Zero-point correction= 0.137707 (Hartree/Particle)
 Thermal correction to Energy= 0.148816
 Thermal correction to Enthalpy= 0.149760
 Thermal correction to Gibbs Free Energy= 0.100002
 Sum of electronic and zero-point Energies= -656.308079
 Sum of electronic and thermal Energies= -656.296971

Sum of electronic and thermal Enthalpies= -656.296027
Sum of electronic and thermal Free Energies= -656.345784

[1MC + H]⁺

H1 1.019516 1.948980 0.000040
C2 1.586902 -0.038189 -0.000003
C3 1.059547 -1.346102 -0.000056
C4 -0.294556 -1.489483 -0.000001
H5 1.708921 -2.208219 -0.000100
H6 -0.748789 -2.472866 -0.000035
N7 0.705663 0.985433 0.000065
C8 -0.694773 0.868738 0.000009
O9 -1.407127 1.826607 -0.000075
N10 -1.151611 -0.448882 0.000096
C11 -2.611549 -0.627244 -0.000014
H12 -3.034998 -0.157781 0.886815
H13 -3.034615 -0.161159 -0.888822
H14 -2.828944 -1.693130 0.002008
N15 2.887659 0.220768 -0.000007
H16 3.553812 -0.535210 -0.000060
H17 3.256715 1.158969 0.000059

Zero-point correction= 0.141261 (Hartree/Particle)
Thermal correction to Energy= 0.149603
Thermal correction to Enthalpy= 0.150547
Thermal correction to Gibbs Free Energy= 0.108086
Sum of electronic and zero-point Energies= -434.465801
Sum of electronic and thermal Energies= -434.457459
Sum of electronic and thermal Enthalpies= -434.456515
Sum of electronic and thermal Free Energies= -434.498976

**Cartesian coordinates for the structures
in Table S1, optimized at ω B97XD/
6-31+G(d,p).**

9MOG⁺

N1 1.540864 -0.777966 -0.002023
 C2 0.057722 0.899800 0.000912
 C3 -1.262756 1.482645 0.000727
 O4 -1.541742 2.658507 0.001037
 N5 -2.249671 0.468398 -0.000064
 H6 -3.203177 0.815473 -0.000372
 C7 -1.997672 -0.874469 -0.000350
 N8 -3.021552 -1.718923 -0.001827
 H9 -3.986613 -1.425407 -0.003151
 H10 -2.817206 -2.708711 -0.001470
 N11 -0.761474 -1.400361 0.001089
 C12 0.217841 -0.520794 0.000662
 C13 2.176393 -2.092013 0.002958
 H14 1.988807 -2.589500 0.955429
 H15 1.777062 -2.689366 -0.816998
 H16 3.246322 -1.938309 -0.131786
 C17 2.263325 0.435928 -0.000758
 O18 3.449798 0.584010 -0.002681
 N19 1.277471 1.452809 0.000861
 H20 1.501771 2.441405 0.000327

Zero-point correction= 0.151699 (Hartree/Particle)
 Thermal correction to Energy= 0.162715
 Thermal correction to Enthalpy= 0.163659
 Thermal correction to Gibbs Free Energy= 0.114360
 Sum of electronic and zero-point Energies= -656.531321
 Sum of electronic and thermal Energies= -656.520305
 Sum of electronic and thermal Enthalpies= -656.519361
 Sum of electronic and thermal Free Energies= -656.568660

¹O₂

O1 0.000000 0.000000 0.602307
 O2 0.000000 0.000000 -0.602307

Zero-point correction= 0.003901 (Hartree/Particle)
 Thermal correction to Energy= 0.006263
 Thermal correction to Enthalpy= 0.007208
 Thermal correction to Gibbs Free Energy= -0.015025
 Sum of electronic and zero-point Energies= -150.211877
 Sum of electronic and thermal Energies= -150.209515
 Sum of electronic and thermal Enthalpies= -150.208570
 Sum of electronic and thermal Free Energies= -150.230803

³O₂

O1 0.000000 0.000000 0.602692
 O2 0.000000 0.000000 -0.602692

Zero-point correction= 0.003920 (Hartree/Particle)
 Thermal correction to Energy= 0.006282
 Thermal correction to Enthalpy= 0.007226
 Thermal correction to Gibbs Free Energy= -0.016045
 Sum of electronic and zero-point Energies= -150.273361
 Sum of electronic and thermal Energies= -150.270999
 Sum of electronic and thermal Enthalpies= -150.270054
 Sum of electronic and thermal Free Energies= -150.293326

9MOG⁺_precursor

C1 -0.053502 0.699824 -0.300204
 C2 0.049501 -0.683595 -0.645663
 C3 1.337029 -1.335683 -0.659858
 C4 2.160244 0.897213 -0.003272
 C5 -2.126156 -0.099236 -0.710687
 H6 3.289638 -0.818137 -0.303571
 H7 -1.446364 -2.086342 -1.148070
 O8 1.565970 -2.493200 -0.920984
 O9 -3.311830 -0.168022 -0.847786
 N10 -1.184637 -1.142973 -0.885534
 N11 -1.359207 1.029828 -0.344191
 N12 0.954317 1.487845 0.009571
 N13 2.356915 -0.418919 -0.313538
 N14 3.212587 1.645273 0.305267
 H15 4.158751 1.296147 0.322588
 H16 3.051094 2.616755 0.531961
 O17 -0.233132 -0.945318 2.329646
 O18 -1.421173 -1.149198 2.360562
 C19 -1.940914 2.335982 -0.051630
 H20 -1.539556 3.078734 -0.741936
 H21 -1.710465 2.615787 0.977045
 H22 -3.018812 2.248545 -0.182668

Zero-point correction= 0.156236 (Hartree/Particle)
 Thermal correction to Energy= 0.171400
 Thermal correction to Enthalpy= 0.172344
 Thermal correction to Gibbs Free Energy= 0.109821
 Sum of electronic and zero-point Energies= -806.808493
 Sum of electronic and thermal Energies= -806.793329
 Sum of electronic and thermal Enthalpies= -806.792385
 Sum of electronic and thermal Free Energies= -806.854907

syn-TS4

C1 0.298804 -0.509923 0.244636
 C2 0.007456 0.936663 -0.067892
 C3 -1.409524 1.427538 -0.141994
 C4 -1.833139 -0.954783 -0.524604
 C5 2.234240 0.550639 -0.464576
 O6 -1.701856 2.590419 -0.067835
 O7 3.329262 0.887730 -0.778428
 N8 1.074049 1.525470 -0.436209
 N9 1.670215 -0.636659 -0.144580
 N10 -0.604139 -1.368074 -0.376141
 N11 -2.266923 0.371543 -0.339851
 N12 -2.781209 -1.812526 -0.902925
 H13 -3.712044 -1.532351 -1.168934
 H14 -2.521607 -2.782676 -1.010740
 O15 -0.575283 0.178230 2.251462
 O16 0.268832 -0.670120 1.719190
 C17 2.419997 -1.891381 -0.066652
 H18 2.611870 -2.152919 0.975145
 H19 3.364363 -1.748135 -0.590669
 H20 1.837961 -2.672293 -0.556460
 H21 1.155522 2.487025 -0.770118
 H22 -3.254652 0.600494 -0.348924

Zero-point correction= 0.157912 (Hartree/Particle)
 Thermal correction to Energy= 0.170594
 Thermal correction to Enthalpy= 0.171539
 Thermal correction to Gibbs Free Energy= 0.118498
 Sum of electronic and zero-point Energies= -806.743958
 Sum of electronic and thermal Energies= -806.731276
 Sum of electronic and thermal Enthalpies= -806.730332
 Sum of electronic and thermal Free Energies= -806.783373

syn-[4-OO-9MOG]⁺

C1 0.257390 -0.520902 0.260415
 C2 -0.019617 0.917941 -0.110636
 C3 -1.441866 1.399955 -0.145918
 C4 -1.875994 -1.001333 -0.424690
 C5 2.173740 0.479213 -0.583504
 O6 -1.746834 2.561157 -0.133365
 O7 3.257956 0.772505 -0.972438
 N8 1.022859 1.451833 -0.613897
 N9 1.631206 -0.666530 -0.104867
 N10 -0.638237 -1.406761 -0.331378
 N11 -2.301264 0.324290 -0.206518
 N12 -2.837860 -1.859493 -0.762520
 H13 -3.778958 -1.580653 -0.991518
 H14 -2.581175 -2.829132 -0.882677
 O15 0.101994 0.634114 2.208587
 O16 0.119838 -0.588587 1.735105
 C17 2.380829 -1.912817 0.051079
 H18 2.542589 -2.123586 1.109306
 H19 3.340751 -1.787752 -0.448805
 H20 1.820350 -2.721660 -0.418859
 H21 1.098388 2.380926 -1.027722
 H22 -3.289394 0.552621 -0.189056

Zero-point correction= 0.158183 (Hartree/Particle)
 Thermal correction to Energy= 0.171636
 Thermal correction to Enthalpy= 0.172580
 Thermal correction to Gibbs Free Energy= 0.117387
 Sum of electronic and zero-point Energies= -806.745551
 Sum of electronic and thermal Energies= -806.732098
 Sum of electronic and thermal Enthalpies= -806.731154
 Sum of electronic and thermal Free Energies= -806.786348

TS4OOH_{N1}

C1 0.301456 -0.459794 0.141862
 C2 0.094890 1.008272 -0.126537
 C3 -1.331490 1.486546 0.031611
 C4 -1.796797 -0.686586 -0.728876
 C5 2.324920 0.543121 -0.328774
 O6 -1.563560 2.636505 0.293112
 O7 3.458156 0.818335 -0.547719
 N8 1.217366 1.558070 -0.384696
 N9 1.695165 -0.626569 -0.021297
 N10 -0.546660 -1.172052 -0.708596
 N11 -2.226316 0.425412 0.002789
 N12 -2.729784 -1.334521 -1.400736
 H13 -3.672572 -0.971390 -1.421249
 H14 -2.510693 -2.201894 -1.871082
 O15 -1.251809 -0.900211 1.873929

O16 0.025561 -0.577600 1.599112
 H17 -1.902960 -0.293822 1.225172
 C18 2.378913 -1.918713 0.060385
 H19 2.278115 -2.327604 1.066403
 H20 3.431996 -1.748466 -0.160699
 H21 1.949301 -2.599704 -0.675834
 H22 1.380276 2.537195 -0.620456

Zero-point correction= 0.151500 (Hartree/Particle)
 Thermal correction to Energy= 0.164091
 Thermal correction to Enthalpy= 0.165035
 Thermal correction to Gibbs Free Energy= 0.112206
 Sum of electronic and zero-point Energies= -806.673845
 Sum of electronic and thermal Energies= -806.661255
 Sum of electronic and thermal Enthalpies= -806.660310
 Sum of electronic and thermal Free Energies= -806.713139

[4-OOH_{N1}-9MOG]⁺

C1 0.300826 -0.490033 0.196239
 C2 0.079298 1.004490 0.063138
 C3 -1.324871 1.550862 -0.013442
 C4 -1.876212 -0.636835 -0.746763
 C5 2.300569 0.571056 -0.303275
 O6 -1.576078 2.666423 0.364291
 O7 3.423309 0.881432 -0.537598
 N8 1.192221 1.576106 -0.185179
 N9 1.684505 -0.626026 -0.129208
 N10 -0.595382 -1.122640 -0.719702
 N11 -2.168619 0.668037 -0.630896
 N12 -2.839378 -1.475953 -1.085756
 H13 -3.781147 -1.127990 -1.203561
 H14 -2.635591 -2.448602 -1.264015
 O15 -1.209002 -0.775168 1.886938
 O16 0.168312 -0.939011 1.525285
 H17 -1.127589 -0.687524 2.849307
 C18 2.382541 -1.910180 -0.197165
 H19 2.511581 -2.328917 0.801552
 H20 3.356462 -1.733122 -0.652491
 H21 1.803213 -2.588918 -0.824763
 H22 1.334403 2.572833 -0.354564

Zero-point correction= 0.155828 (Hartree/Particle)
 Thermal correction to Energy= 0.169740
 Thermal correction to Enthalpy= 0.170684
 Thermal correction to Gibbs Free Energy= 0.114608
 Sum of electronic and zero-point Energies= -806.710153
 Sum of electronic and thermal Energies= -806.696241
 Sum of electronic and thermal Enthalpies= -806.695297
 Sum of electronic and thermal Free Energies= -806.751372

anti-TS5

C1 -0.338196 0.622423 -0.188874
 C2 -0.142935 -0.821565 -0.100394
 C3 1.131828 -1.358523 -0.612138
 C4 1.871428 0.970922 -0.364287
 C5 -2.362384 -0.388631 -0.171634
 H6 3.048445 -0.669567 -0.859471
 H7 -1.580848 -2.370945 -0.236546

O8 1.349077 -2.496146 -0.930501
 O9 -3.546066 -0.526632 -0.168805
 N10 -1.369894 -1.381533 -0.209326
 N11 -1.652148 0.853126 -0.157330
 N12 0.635631 1.493823 -0.221020
 N13 2.114241 -0.353195 -0.620436
 N14 2.891760 1.808344 -0.322555
 H15 3.855490 1.514557 -0.384103
 H16 2.693666 2.787375 -0.163806
 O17 0.266212 -0.891065 1.749702
 O18 1.185410 -0.168095 2.155044
 C19 -2.316248 2.152752 -0.162535
 H20 -2.157018 2.645249 -1.122929
 H21 -1.915086 2.765660 0.644993
 H22 -3.379813 1.974954 -0.007818

Zero-point correction= 0.157591 (Hartree/Particle)
 Thermal correction to Energy= 0.170723
 Thermal correction to Enthalpy= 0.171667
 Thermal correction to Gibbs Free Energy= 0.117632
 Sum of electronic and zero-point Energies= -806.786846
 Sum of electronic and thermal Energies= -806.773714
 Sum of electronic and thermal Enthalpies= -806.772770
 Sum of electronic and thermal Free Energies= -806.826805

***anti*-[5-OO-9MOG]⁺**

C1 -0.317849 0.669276 -0.000312
 C2 -0.111440 -0.821699 0.118339
 C3 1.117621 -1.265912 -0.665108
 C4 1.879863 1.024868 -0.284910
 C5 -2.335277 -0.352184 -0.186416
 H6 2.987818 -0.540031 -1.098115
 H7 -1.594125 -2.320597 -0.235858
 O8 1.269191 -2.355364 -1.135610
 O9 -3.517163 -0.447899 -0.292277
 N10 -1.361785 -1.336329 -0.224218
 N11 -1.617534 0.899067 -0.042271
 N12 0.656254 1.535178 -0.043692
 N13 2.088648 -0.258883 -0.720663
 N14 2.912369 1.837054 -0.183903
 H15 3.868031 1.538529 -0.316094
 H16 2.738142 2.796107 0.087702
 O17 0.134370 -1.142204 1.560986
 O18 1.221761 -0.608823 2.032585
 C19 -2.278807 2.197306 -0.121983
 H20 -2.099650 2.646297 -1.100655
 H21 -1.890367 2.844751 0.664111
 H22 -3.345462 2.026713 0.018998

Zero-point correction= 0.159376 (Hartree/Particle)
 Thermal correction to Energy= 0.172428
 Thermal correction to Enthalpy= 0.173372
 Thermal correction to Gibbs Free Energy= 0.119659
 Sum of electronic and zero-point Energies= -806.793717
 Sum of electronic and thermal Energies= -806.780664
 Sum of electronic and thermal Enthalpies= -806.779720
 Sum of electronic and thermal Free Energies= -806.833434

TS5OOH_{N1}

C1 -0.374667 0.714432 0.028756
 C2 -0.083734 -0.785872 0.031877
 C3 1.158258 -1.048265 -0.870124
 C4 1.815101 1.117584 -0.248622
 C5 -2.345907 -0.411976 -0.082440
 H6 2.145954 -0.791678 0.978123
 H7 -1.483432 -2.330612 -0.374382
 O8 1.198343 -2.001783 -1.590700
 O9 -3.518044 -0.594762 -0.167171
 N10 -1.315030 -1.358077 -0.149596
 N11 -1.700129 0.856225 0.067919
 N12 0.536223 1.617991 -0.059304
 N13 2.157620 -0.154214 -0.548380
 N14 2.785802 1.997893 -0.113130
 H15 3.740212 1.731362 -0.315445
 H16 2.564922 2.958215 0.112711
 O17 0.343537 -1.190881 1.452695
 O18 1.621440 -1.188082 1.785355
 C19 -2.428064 2.122244 0.026807
 H20 -2.283490 2.600987 -0.943369
 H21 -2.060690 2.770640 0.822181
 H22 -3.483011 1.897547 0.178661

Zero-point correction= 0.155160 (Hartree/Particle)
 Thermal correction to Energy= 0.167810
 Thermal correction to Enthalpy= 0.168754
 Thermal correction to Gibbs Free Energy= 0.115720
 Sum of electronic and zero-point Energies= -806.727117
 Sum of electronic and thermal Energies= -806.714467
 Sum of electronic and thermal Enthalpies= -806.713523
 Sum of electronic and thermal Free Energies= -806.766556

[5-OOH_{N1}-9MOG]⁺

C1 -0.312676 0.683236 0.126456
 C2 -0.127257 -0.831761 0.200252
 C3 1.200186 -1.129628 -0.923857
 C4 1.860894 1.040592 -0.310771
 C5 -2.338201 -0.315440 -0.128445
 H6 1.811505 -1.451658 2.420981
 H7 -1.627146 -2.299258 -0.135812
 O8 1.074092 -2.192611 -1.444091
 O9 -3.515663 -0.422714 -0.273302
 N10 -1.370236 -1.320618 -0.158318
 N11 -1.627286 0.908150 0.075335
 N12 0.637851 1.545753 0.047066
 N13 2.086397 -0.168152 -0.858637
 N14 2.891012 1.851773 -0.192710
 H15 3.809849 1.554541 -0.491052
 H16 2.752157 2.787281 0.163293
 O17 0.266256 -1.379501 1.396164
 O18 1.434061 -0.740550 1.877852
 C19 -2.262215 2.217435 -0.055193
 H20 -2.034273 2.647041 -1.032626
 H21 -1.894283 2.870986 0.735304
 H22 -3.336337 2.069120 0.047133

Zero-point correction= 0.156847 (Hartree/Particle)
 Thermal correction to Energy= 0.170741
 Thermal correction to Enthalpy= 0.171685
 Thermal correction to Gibbs Free Energy= 0.115852
 Sum of electronic and zero-point Energies= -806.756099
 Sum of electronic and thermal Energies= -806.742205
 Sum of electronic and thermal Enthalpies= -806.741261
 Sum of electronic and thermal Free Energies= -806.797094

TS5OOHN₂

C1 0.363103 -0.611127 -0.324220
 C2 0.002290 0.747184 0.235751
 C3 -1.039778 1.377159 -0.700566
 C4 -1.799299 -0.901712 -0.563106
 C5 2.279539 0.463153 0.232212
 H6 -3.017442 0.710975 -0.975174
 H7 1.373290 2.312439 0.702494
 O8 -1.080707 2.503143 -1.082841
 O9 3.446309 0.658089 0.356032
 N10 1.219754 1.334237 0.496244
 N11 1.682995 -0.743988 -0.272031
 N12 -0.555952 -1.421645 -0.739902
 N13 -2.052314 0.401267 -0.888789
 N14 -2.729420 -1.523500 0.166518
 H15 -2.199714 -0.914540 1.382946
 H16 -2.476128 -2.510221 0.275727
 O17 -0.928151 0.638641 1.465738
 O18 -1.214308 -0.610780 1.856075
 C19 2.462220 -1.895918 -0.716559
 H20 2.325120 -2.041125 -1.789057
 H21 2.137429 -2.784080 -0.172838
 H22 3.508416 -1.683227 -0.499482

Zero-point correction= 0.152112 (Hartree/Particle)
 Thermal correction to Energy= 0.164425
 Thermal correction to Enthalpy= 0.165370
 Thermal correction to Gibbs Free Energy= 0.113615
 Sum of electronic and zero-point Energies= -806.688621
 Sum of electronic and thermal Energies= -806.676307
 Sum of electronic and thermal Enthalpies= -806.675363
 Sum of electronic and thermal Free Energies= -806.727118

[5-OOHN₂-9MOG]^{•+}

C1 -0.339060 0.669496 0.139093
 C2 -0.046739 -0.825328 0.095540
 C3 1.217903 -1.088506 -0.742991
 C4 1.793382 1.239188 -0.248166
 C5 -2.289584 -0.420383 -0.264559
 H6 2.962602 -0.094003 -1.273613
 H7 -1.460911 -2.324938 -0.474787
 O8 1.470817 -2.145031 -1.246273
 O9 -3.463646 -0.531452 -0.415611
 N10 -1.271087 -1.333573 -0.397267
 N11 -1.628556 0.854140 0.054794
 N12 0.601036 1.602889 0.219281
 N13 2.063987 0.022921 -0.811994
 N14 2.812839 2.128877 -0.310090
 H15 1.720052 -1.685539 2.308012

H16 2.583570 2.942399 0.271616
 O17 0.113303 -1.344256 1.406258
 O18 1.368299 -0.874080 1.909963
 C19 -2.359836 2.117034 0.084513
 H20 -2.324148 2.583269 -0.902148
 H21 -1.902175 2.770402 0.826571
 H22 -3.393116 1.891175 0.346000

Zero-point correction= 0.156404 (Hartree/Particle)
 Thermal correction to Energy= 0.170079
 Thermal correction to Enthalpy= 0.171023
 Thermal correction to Gibbs Free Energy= 0.115428
 Sum of electronic and zero-point Energies= -806.743905
 Sum of electronic and thermal Energies= -806.730231
 Sum of electronic and thermal Enthalpies= -806.729286
 Sum of electronic and thermal Free Energies= -806.784881

syn-TS5

C1 -0.121761 0.719968 -0.124532
 C2 -0.027382 -0.737239 -0.223380
 C3 1.277974 -1.303216 -0.605594
 C4 2.107941 0.942164 -0.025685
 C5 -2.188724 -0.130711 -0.484442
 H6 3.244710 -0.729608 -0.506157
 H7 -1.524303 -2.136156 -0.746204
 O8 1.484834 -2.410406 -1.019934
 O9 -3.367453 -0.171795 -0.644070
 N10 -1.254053 -1.175744 -0.575231
 N11 -1.411830 1.039916 -0.192188
 N12 0.897962 1.525962 0.046968
 N13 2.306622 -0.373357 -0.353886
 N14 3.164730 1.702371 0.206781
 H15 4.113403 1.357972 0.193784
 H16 3.006640 2.676859 0.426306
 O17 0.097040 -1.049134 1.638856
 O18 -1.044136 -1.300020 2.037406
 C19 -1.996815 2.372492 -0.077641
 H20 -1.771124 2.954414 -0.972668
 H21 -1.588768 2.865118 0.804755
 H22 -3.074257 2.247458 0.022657

Zero-point correction= 0.157565 (Hartree/Particle)
 Thermal correction to Energy= 0.170895
 Thermal correction to Enthalpy= 0.171839
 Thermal correction to Gibbs Free Energy= 0.116656
 Sum of electronic and zero-point Energies= -806.789854
 Sum of electronic and thermal Energies= -806.776524
 Sum of electronic and thermal Enthalpies= -806.775580
 Sum of electronic and thermal Free Energies= -806.830763

syn-[5-OO-9MOG]^{•+}

C1 -0.151646 0.692190 -0.044490
 C2 -0.041019 -0.811764 0.049596
 C3 1.244110 -1.304555 -0.597658
 C4 2.081071 0.936391 -0.061698
 C5 -2.195936 -0.210948 -0.430671
 H6 3.196859 -0.686345 -0.736019
 H7 -1.568679 -2.213046 -0.456285

O8 1.394469 -2.374992 -1.107811
 O9 -3.368708 -0.233966 -0.629359
 N10 -1.275736 -1.245395 -0.426494
 N11 -1.421811 0.997508 -0.202588
 N12 0.868931 1.505509 0.050948
 N13 2.276589 -0.365050 -0.452736
 N14 3.138901 1.696163 0.151983
 H15 4.087493 1.352177 0.114574
 H16 2.985134 2.666333 0.394572
 O17 0.200092 -1.148869 1.496574
 O18 -0.837755 -0.864043 2.222968
 C19 -2.009727 2.330825 -0.274210
 H20 -1.768507 2.792079 -1.233478
 H21 -1.617718 2.935462 0.543428
 H22 -3.088602 2.214319 -0.178761

Zero-point correction= 0.158914 (Hartree/Particle)
 Thermal correction to Energy= 0.172221
 Thermal correction to Enthalpy= 0.173165
 Thermal correction to Gibbs Free Energy= 0.118139
 Sum of electronic and zero-point Energies= -806.794062
 Sum of electronic and thermal Energies= -806.780756
 Sum of electronic and thermal Enthalpies= -806.779811
 Sum of electronic and thermal Free Energies= -806.834837

TS5OOH_{N7}

C1 -0.178164 0.805939 0.186237
 C2 -0.134293 -0.701710 0.030778
 C3 1.118319 -1.092195 -0.826027
 C4 2.046504 1.017859 0.042862
 C5 -2.218028 -0.029321 -0.348341
 H6 3.053249 -0.465965 -1.014394
 H7 -1.188618 -2.364964 0.916214
 O8 1.216505 -2.074284 -1.487573
 O9 -3.380842 0.031838 -0.604032
 N10 -1.381186 -1.138100 -0.325001
 N11 -1.432913 1.158072 0.029712
 N12 0.867876 1.575354 0.351510
 N13 2.163181 -0.181585 -0.618241
 N14 3.146810 1.694111 0.315820
 H15 4.075947 1.345821 0.128914
 H16 3.049793 2.599779 0.756449
 O17 0.293442 -1.301496 1.320983
 O18 -0.392635 -2.458766 1.524425
 C19 -1.979503 2.509247 0.043050
 H20 -1.534963 3.094574 -0.764023
 H21 -1.767420 2.977127 1.004949
 H22 -3.055131 2.421410 -0.106489

Zero-point correction= 0.154561 (Hartree/Particle)
 Thermal correction to Energy= 0.167547
 Thermal correction to Enthalpy= 0.168491
 Thermal correction to Gibbs Free Energy= 0.114481
 Sum of electronic and zero-point Energies= -806.728736
 Sum of electronic and thermal Energies= -806.715750
 Sum of electronic and thermal Enthalpies= -806.714806
 Sum of electronic and thermal Free Energies= -806.768816

[5-OOH_{N7}-9MOG]⁺

C1 -0.149552 0.681733 -0.038834
 C2 -0.050730 -0.833039 0.057668
 C3 1.231107 -1.296050 -0.654970
 C4 2.073084 0.929115 -0.034200
 C5 -2.171284 -0.231603 -0.461026
 H6 3.183783 -0.667916 -0.764726
 H7 -1.235797 -1.494687 2.586063
 O8 1.392195 -2.334432 -1.215791
 O9 -3.351358 -0.264725 -0.650100
 N10 -1.299619 -1.342354 -0.438921
 N11 -1.417174 0.982223 -0.259460
 N12 0.858245 1.502674 0.063062
 N13 2.262959 -0.351380 -0.478396
 N14 3.128324 1.674985 0.232165
 H15 4.075767 1.327036 0.203301
 H16 2.973778 2.636806 0.505235
 O17 0.185464 -1.252580 1.386291
 O18 -0.838130 -0.692834 2.209976
 C19 -1.999042 2.315054 -0.370783
 H20 -1.782974 2.732329 -1.356333
 H21 -1.574865 2.951671 0.405639
 H22 -3.075705 2.217040 -0.238476

Zero-point correction= 0.157370 (Hartree/Particle)
 Thermal correction to Energy= 0.170925
 Thermal correction to Enthalpy= 0.171870
 Thermal correction to Gibbs Free Energy= 0.116427
 Sum of electronic and zero-point Energies= -806.749366
 Sum of electronic and thermal Energies= -806.735810
 Sum of electronic and thermal Enthalpies= -806.734866
 Sum of electronic and thermal Free Energies= -806.790309

TSOOH_{N2}

C1 0.652835 -0.455231 -0.334812
 C2 0.679315 0.971382 -0.089782
 C3 -0.533395 1.796590 -0.272065
 C4 -1.562807 -0.389407 -0.833622
 C5 2.741435 0.117630 0.300499
 O6 -0.558678 2.991312 -0.099692
 O7 3.891244 0.124939 0.601808
 N8 1.878675 1.303738 0.278365
 N9 1.911263 -0.923315 -0.093654
 N10 -0.398885 -1.117267 -0.684269
 N11 -1.577218 0.999655 -0.681552
 N12 -2.691422 -0.950813 -1.133296
 H13 -3.450774 -0.878738 0.128621
 H14 -2.552615 -1.947284 -1.307279
 O15 -3.553527 -0.836382 1.201894
 O16 -2.393021 -0.587075 1.667209
 C17 2.346216 -2.316814 -0.199293
 H18 1.765565 -2.930418 0.490276
 H19 3.402461 -2.354098 0.064228
 H20 2.204478 -2.663988 -1.223161
 H21 2.206110 2.238204 0.520162
 H22 -2.461859 1.465070 -0.867314

Zero-point correction= 0.152009 (Hartree/Particle)
 Thermal correction to Energy= 0.165478
 Thermal correction to Enthalpy= 0.166423
 Thermal correction to Gibbs Free Energy= 0.110111
 Sum of electronic and zero-point Energies= -806.723520
 Sum of electronic and thermal Energies= -806.710050
 Sum of electronic and thermal Enthalpies= -806.709106
 Sum of electronic and thermal Free Energies= -806.765417

[9MOG - H_{N2}]⁺ + HOO^{*}

C1 0.629754 -0.480496 -0.415865
 C2 0.519649 0.955511 -0.152593
 C3 -0.748171 1.694426 -0.430771
 C4 -1.585669 -0.582344 -0.948627
 C5 2.629344 0.260918 0.333224
 O6 -0.841490 2.886990 -0.278002
 O7 3.750193 0.385299 0.698260
 N8 1.649602 1.381987 0.279981
 N9 1.921757 -0.831885 -0.126147
 N10 -0.333564 -1.208418 -0.827320
 N11 -1.688474 0.824707 -0.899458
 N12 -2.665152 -1.234119 -1.096823
 H13 -3.388619 -0.956259 0.811430
 H14 -2.476213 -2.232547 -1.186182
 O15 -3.157054 -0.727425 1.746434
 O16 -1.877544 -0.465007 1.753648
 C17 2.480471 -2.183112 -0.220940
 H18 1.994788 -2.830250 0.510374
 H19 3.547265 -2.114909 -0.012418
 H20 2.320382 -2.565269 -1.229223
 H21 1.879565 2.342399 0.540739
 H22 -2.611470 1.202653 -1.095638

Zero-point correction= 0.156160 (Hartree/Particle)
 Thermal correction to Energy= 0.170640
 Thermal correction to Enthalpy= 0.171584
 Thermal correction to Gibbs Free Energy= 0.112777
 Sum of electronic and zero-point Energies= -806.724327
 Sum of electronic and thermal Energies= -806.709847
 Sum of electronic and thermal Enthalpies= -806.708903
 Sum of electronic and thermal Free Energies= -806.767710

TS4OOH_{N2}

C1 0.285525 -0.472236 -0.158897
 C2 0.110687 0.980538 -0.126091
 C3 -1.259428 1.572363 -0.158632
 C4 -1.909218 -0.766907 -0.664953
 C5 2.329026 0.514726 -0.204499
 H6 -3.155867 0.865713 -0.469645
 H7 1.458394 2.541921 -0.028787
 O8 -1.466119 2.748066 0.004140
 O9 3.490881 0.760359 -0.201691
 N10 1.266690 1.544145 -0.109617
 N11 1.644003 -0.676395 -0.312772
 N12 -0.670703 -1.288116 -0.649511
 N13 -2.177799 0.592214 -0.428351
 N14 -2.971483 -1.500179 -0.929400
 H15 -1.192817 -1.736763 2.173718

H16 -2.677181 -2.457282 -1.139659
 O17 -1.182292 -0.772260 2.042939
 O18 0.079273 -0.501690 1.617210
 C19 2.302229 -1.981505 -0.366527
 H20 1.826411 -2.586425 -1.137982
 H21 2.230671 -2.473157 0.605085
 H22 3.348559 -1.813363 -0.618357

Zero-point correction= 0.154724 (Hartree/Particle)
 Thermal correction to Energy= 0.168038
 Thermal correction to Enthalpy= 0.168982
 Thermal correction to Gibbs Free Energy= 0.114254
 Sum of electronic and zero-point Energies= -806.700446
 Sum of electronic and thermal Energies= -806.687132
 Sum of electronic and thermal Enthalpies= -806.686188
 Sum of electronic and thermal Free Energies= -806.740915

[4-OOH_{N2}-9MOG]⁺

C1 0.296442 -0.503170 0.186686
 C2 0.008660 0.976748 0.037439
 C3 -1.403817 1.491040 -0.020054
 C4 -1.823751 -0.827171 -0.756356
 C5 2.242513 0.643664 -0.333039
 H6 -3.209374 0.708352 -0.590375
 H7 1.187738 2.615448 -0.327369
 O8 -1.686125 2.635834 0.221883
 O9 3.350261 1.009735 -0.551562
 N10 1.090268 1.608800 -0.182083
 N11 1.663841 -0.579004 -0.225425
 N12 -0.614194 -1.313181 -0.554707
 N13 -2.227759 0.489260 -0.446173
 N14 -2.800246 -1.575476 -1.276991
 H15 -1.176444 -1.559625 2.472464
 H16 -2.415027 -2.491542 -1.523930
 O17 -1.028220 -0.690609 2.068588
 O18 0.299277 -0.833620 1.569047
 C19 2.429272 -1.827781 -0.258381
 H20 1.840166 -2.578082 -0.785324
 H21 2.659215 -2.162194 0.754305
 H22 3.352894 -1.635857 -0.803529

Zero-point correction= 0.156145 (Hartree/Particle)
 Thermal correction to Energy= 0.169654
 Thermal correction to Enthalpy= 0.170599
 Thermal correction to Gibbs Free Energy= 0.115526
 Sum of electronic and zero-point Energies= -806.713227
 Sum of electronic and thermal Energies= -806.699717
 Sum of electronic and thermal Enthalpies= -806.698773
 Sum of electronic and thermal Free Energies= -806.753845

T5OOH_{N7}

C1 0.637450 0.816441 -0.038087
 C2 0.090813 -0.510218 -0.330573
 C3 1.000978 -1.665335 -0.315230
 C4 2.720981 0.026792 0.231620
 C5 -1.554273 0.921449 -0.448471
 H6 2.997324 -2.016284 0.012390
 H7 -2.255877 -1.327078 -0.056683

O8 0.716013 -2.814997 -0.507625
 O9 -2.664817 1.343313 -0.547647
 N10 -1.173778 -0.459757 -0.615867
 N11 -0.388500 1.666831 -0.115741
 N12 1.890874 1.091247 0.220669
 N13 2.324152 -1.256851 -0.014642
 N14 3.993990 0.263308 0.499084
 H15 4.701452 -0.456171 0.532501
 H16 4.269139 1.220024 0.678545
 O17 -3.821957 -0.888605 0.943975
 O18 -3.016759 -1.780597 0.531995
 C19 -0.367267 3.110384 0.099955
 H20 0.165425 3.597444 -0.718156
 H21 0.124285 3.324755 1.049161
 H22 -1.400855 3.453875 0.126852

Zero-point correction= 0.151361 (Hartree/Particle)
 Thermal correction to Energy= 0.165402
 Thermal correction to Enthalpy= 0.166346
 Thermal correction to Gibbs Free Energy= 0.108119
 Sum of electronic and zero-point Energies= -806.743131
 Sum of electronic and thermal Energies= -806.729090
 Sum of electronic and thermal Enthalpies= -806.728146
 Sum of electronic and thermal Free Energies= -806.786373

[9MOG - H_{N7}]⁺ + HOO[•]

C1 0.350810 0.677339 -0.258507
 C2 0.316403 -0.798807 -0.455309
 C3 1.578573 -1.555597 -0.233330
 C4 2.523918 0.671668 0.303251
 C5 -1.675445 -0.053639 -0.820408
 H6 3.512980 -1.148080 0.321198
 H7 -3.723460 -0.649268 0.508700
 O8 1.747808 -2.732756 -0.345363
 O9 -2.828233 -0.027475 -1.132855
 N10 -0.833314 -1.236892 -0.773453
 N11 -0.878707 1.097676 -0.522503
 N12 1.388685 1.381136 0.100772
 N13 2.627637 -0.681003 0.150851
 N14 3.590165 1.356141 0.671312
 H15 4.490328 0.935261 0.851920
 H16 3.494522 2.357602 0.780218
 O17 -2.228897 -0.490814 1.577101
 O18 -3.508805 -0.700289 1.472952
 C19 -1.406912 2.452727 -0.411849
 H20 -0.671090 3.152892 -0.806723
 H21 -1.619018 2.678906 0.634778
 H22 -2.324587 2.501814 -0.996720

Zero-point correction= 0.156625 (Hartree/Particle)
 Thermal correction to Energy= 0.171081
 Thermal correction to Enthalpy= 0.172025
 Thermal correction to Gibbs Free Energy= 0.113752
 Sum of electronic and zero-point Energies= -806.758782
 Sum of electronic and thermal Energies= -806.744326
 Sum of electronic and thermal Enthalpies= -806.743382
 Sum of electronic and thermal Free Energies= -806.801655

TS4OOH_{N7}

C1 0.333623 -0.477672 0.025981
 C2 0.143705 1.001114 -0.182286
 C3 -1.251441 1.518050 -0.239473
 C4 -1.873242 -0.860489 -0.557526
 C5 2.278372 0.605889 -0.366182
 O6 -1.616346 2.651186 -0.158539
 O7 3.439736 0.833783 -0.486174
 N8 1.220274 1.631899 -0.393134
 N9 1.673587 -0.650155 -0.221843
 N10 -0.610212 -1.357908 -0.466015
 N11 -2.183425 0.454553 -0.427184
 N12 -2.819969 -1.744087 -0.813312
 H13 -3.791537 -1.500935 -0.951694
 H14 -2.550757 -2.718237 -0.879980
 O15 -0.776481 0.064054 2.240570
 O16 0.033763 -0.840653 1.590897
 C17 2.413027 -1.907440 -0.165752
 H18 2.579256 -2.214154 0.868600
 H19 3.373384 -1.743738 -0.653798
 H20 1.856097 -2.675316 -0.703660
 H21 -0.187543 0.806263 2.473393
 H22 -3.150326 0.762326 -0.485049

Zero-point correction= 0.155630 (Hartree/Particle)
 Thermal correction to Energy= 0.169038
 Thermal correction to Enthalpy= 0.169982
 Thermal correction to Gibbs Free Energy= 0.114941
 Sum of electronic and zero-point Energies= -806.706420
 Sum of electronic and thermal Energies= -806.693012
 Sum of electronic and thermal Enthalpies= -806.692068
 Sum of electronic and thermal Free Energies= -806.747110

[4-OOH_{N7}-9MOG]^{•+}

C1 0.257861 -0.515127 0.139806
 C2 -0.007476 1.011158 -0.154052
 C3 -1.417127 1.484133 -0.026563
 C4 -1.969115 -0.859678 -0.503387
 C5 2.106551 0.638748 -0.623669
 H6 1.082620 -0.466556 2.898312
 O7 -1.788847 2.598725 0.168053
 O8 3.219091 0.903656 -0.954195
 N9 1.002300 1.616105 -0.575475
 N10 1.608676 -0.594974 -0.231898
 N11 -0.662016 -1.184908 -0.706486
 N12 -2.333350 0.402830 -0.180952
 N13 -2.868967 -1.798998 -0.714639
 H14 -3.860899 -1.650608 -0.586481
 H15 -2.555304 -2.718992 -0.998142
 O16 0.533072 0.087445 2.322678
 O17 -0.056789 -0.882527 1.460058
 H18 -3.313078 0.669592 -0.149076
 C19 2.412574 -1.804459 -0.144953
 H20 2.547393 -2.108324 0.895676
 H21 3.386236 -1.583319 -0.581619
 H22 1.934698 -2.609223 -0.708361

Zero-point correction= 0.155677 (Hartree/Particle)
 Thermal correction to Energy= 0.169632
 Thermal correction to Enthalpy= 0.170576
 Thermal correction to Gibbs Free Energy= 0.114064
 Sum of electronic and zero-point Energies= -806.717951
 Sum of electronic and thermal Energies= -806.703996
 Sum of electronic and thermal Enthalpies= -806.703052
 Sum of electronic and thermal Free Energies= -806.759564

TS24

C1 0.310731 -0.475991 0.059882
 C2 0.212323 1.015871 0.010751
 C3 -1.131477 1.681849 0.023058
 C4 -1.855003 -0.633644 -0.355354
 C5 2.411566 0.441507 -0.145108
 H6 1.614328 2.514256 -0.184384
 O7 -1.257427 2.872194 0.150615
 O8 3.574234 0.655332 -0.253017
 N9 1.384172 1.524761 -0.096299
 N10 1.690356 -0.717823 -0.068142
 N11 -0.596271 -0.932624 -0.899543
 N12 -2.909565 -1.328251 -0.846871
 H13 -3.821280 -1.186926 -0.434948
 H14 -2.712878 -2.277634 -1.133246
 O15 -0.180971 -0.854252 1.391764
 O16 -1.488881 -1.168518 1.199219
 C17 2.285934 -2.053522 -0.133577
 H18 2.135889 -2.573244 0.813483
 H19 3.352232 -1.928783 -0.318747
 H20 1.830236 -2.607915 -0.955278
 N21 -2.125719 0.749703 -0.132441
 H22 -3.079421 1.095425 -0.150370

Zero-point correction= 0.156006 (Hartree/Particle)
 Thermal correction to Energy= 0.168492
 Thermal correction to Enthalpy= 0.169436
 Thermal correction to Gibbs Free Energy= 0.117169
 Sum of electronic and zero-point Energies= -806.699287
 Sum of electronic and thermal Energies= -806.686801
 Sum of electronic and thermal Enthalpies= -806.685857
 Sum of electronic and thermal Free Energies= -806.738124

[2,4-OO-9MOG]⁺

C1 0.305427 -0.472600 0.036193
 C2 0.250367 1.037576 0.007982
 C3 -1.089554 1.722187 0.011798
 C4 -1.874898 -0.650903 -0.209571
 C5 2.437615 0.390206 -0.120895
 H6 1.692300 2.498426 -0.020747
 O7 -1.186889 2.921594 0.080280
 O8 3.604736 0.586242 -0.185679
 N9 1.430316 1.511120 -0.033884
 N10 1.681446 -0.744884 -0.121837
 N11 -0.642592 -0.924266 -0.935859
 N12 -3.001003 -1.267200 -0.750042
 H13 -3.798909 -1.277029 -0.123154
 H14 -2.805296 -2.196382 -1.103846
 O15 -0.186742 -0.833324 1.329529

O16 -1.559791 -1.186627 1.098079
 C17 2.247262 -2.096074 -0.163235
 H18 2.057589 -2.604999 0.782721
 H19 3.320674 -1.998304 -0.321234
 H20 1.802394 -2.644467 -0.994509
 N21 -2.079347 0.795421 -0.139722
 H22 -3.018321 1.145985 -0.301113

Zero-point correction= 0.158102 (Hartree/Particle)
 Thermal correction to Energy= 0.170649
 Thermal correction to Enthalpy= 0.171593
 Thermal correction to Gibbs Free Energy= 0.119087
 Sum of electronic and zero-point Energies= -806.709080
 Sum of electronic and thermal Energies= -806.696533
 Sum of electronic and thermal Enthalpies= -806.695589
 Sum of electronic and thermal Free Energies= -806.748095

[9MOG - H][•]

N1 1.529427 -0.778624 -0.002273
 C2 0.005568 0.872323 0.000746
 C3 -1.338317 1.440687 0.001003
 O4 -1.507430 2.657670 0.001839
 N5 -2.341036 0.502813 0.000021
 C6 -2.043437 -0.781779 -0.000344
 N7 -3.062640 -1.663321 -0.002416
 H8 -4.006791 -1.314896 -0.003781
 H9 -2.871343 -2.650384 -0.002285
 N10 -0.793530 -1.401412 0.001297
 C11 0.177615 -0.536530 0.000749
 C12 2.165742 -2.080335 0.003528
 H13 1.967685 -2.594062 0.946760
 H14 1.781946 -2.680984 -0.823097
 H15 3.237976 -1.924365 -0.114443
 C16 2.225251 0.432303 -0.001129
 O17 3.422557 0.597156 -0.002633
 N18 1.235688 1.430079 -0.000012
 H19 1.439622 2.419329 -0.000446

Zero-point correction= 0.138109 (Hartree/Particle)
 Thermal correction to Energy= 0.149229
 Thermal correction to Enthalpy= 0.150173
 Thermal correction to Gibbs Free Energy= 0.100388
 Sum of electronic and zero-point Energies= -656.164667
 Sum of electronic and thermal Energies= -656.153547
 Sum of electronic and thermal Enthalpies= -656.152603
 Sum of electronic and thermal Free Energies= -656.202388

[9MOG - H][•]_precursor

C1 -1.143932 1.538201 -0.450258
 C2 0.177996 0.926390 -0.360592
 C3 -1.897800 -0.650786 -0.731927
 C4 2.371057 0.412087 -0.152951
 N5 -2.162714 0.638008 -0.640640
 N6 1.412428 1.439366 -0.174112
 N7 1.651542 -0.769109 -0.347722
 N8 -0.670206 -1.309658 -0.660663
 C9 0.315435 -0.481798 -0.477219
 N10 -2.932248 -1.492395 -0.923802

H11 -2.768038 -2.482380 -0.985592
 H12 -3.862744 -1.113243 -0.980495
 O13 -1.282535 2.755088 -0.355150
 O14 -1.300796 -0.760633 2.591924
 O15 -0.449244 0.087055 2.491414
 C16 2.250602 -2.087485 -0.391776
 H17 3.321354 -1.967958 -0.227075
 H18 1.820915 -2.717964 0.389315
 H19 2.073288 -2.548160 -1.365772
 O20 3.563372 0.534796 0.001249
 H21 1.637106 2.416119 -0.048967

Zero-point correction= 0.142829 (Hartree/Particle)
 Thermal correction to Energy= 0.157964
 Thermal correction to Enthalpy= 0.158908
 Thermal correction to Gibbs Free Energy= 0.097318
 Sum of electronic and zero-point Energies= -806.440885
 Sum of electronic and thermal Energies= -806.425751
 Sum of electronic and thermal Enthalpies= -806.424807
 Sum of electronic and thermal Free Energies= -806.486397

anti-TS5 (neutral radical)

C1 -0.287445 0.621676 -0.226522
 C2 -0.093112 -0.810106 -0.138821
 C3 1.213144 -1.352623 -0.595717
 C4 1.928989 0.850834 -0.420200
 C5 -2.317880 -0.381582 -0.187621
 H6 -1.521979 -2.357798 -0.267932
 O7 1.325093 -2.536375 -0.872133
 O8 -3.511844 -0.541967 -0.182583
 N9 -1.325596 -1.368608 -0.224866
 N10 -1.631094 0.845459 -0.176697
 N11 0.675408 1.474448 -0.294173
 N12 2.212681 -0.421529 -0.621849
 N13 2.942964 1.725842 -0.388931
 H14 3.885879 1.378580 -0.453976
 H15 2.756848 2.701627 -0.230298
 O16 0.253097 -0.822365 1.814216
 O17 1.078593 -0.009569 2.247844
 C18 -2.284585 2.139176 -0.193475
 H19 -2.105819 2.640159 -1.147422
 H20 -1.896887 2.755787 0.619165
 H21 -3.352757 1.970324 -0.058530

Zero-point correction= 0.144063 (Hartree/Particle)
 Thermal correction to Energy= 0.157293
 Thermal correction to Enthalpy= 0.158237
 Thermal correction to Gibbs Free Energy= 0.103709
 Sum of electronic and zero-point Energies= -806.427172
 Sum of electronic and thermal Energies= -806.413943
 Sum of electronic and thermal Enthalpies= -806.412999
 Sum of electronic and thermal Free Energies= -806.467527

anti-[5-OO-9MOG - H]•

C1 -0.266498 0.677165 -0.002368
 C2 -0.056953 -0.806087 0.126765
 C3 1.176179 -1.248217 -0.679101
 C4 1.932875 0.908381 -0.351255

C5 -2.288887 -0.335363 -0.177782
 H6 -1.525064 -2.293455 -0.343918
 O7 1.195027 -2.362001 -1.163235
 O8 -3.478321 -0.447820 -0.323823
 N9 -1.322305 -1.316843 -0.197005
 N10 -1.598732 0.897228 0.004022
 N11 0.683633 1.523660 -0.147376
 N12 2.182522 -0.331659 -0.719355
 N13 2.954375 1.760609 -0.240580
 H14 3.891447 1.419238 -0.382523
 H15 2.780948 2.722674 -0.001717
 O16 0.169452 -1.139269 1.568736
 O17 1.143428 -0.477465 2.120925
 C18 -2.240942 2.189967 -0.132830
 H19 -2.003221 2.633595 -1.103027
 H20 -1.895892 2.852163 0.662357
 H21 -3.315996 2.032180 -0.050509

Zero-point correction= 0.145824 (Hartree/Particle)
 Thermal correction to Energy= 0.159052
 Thermal correction to Enthalpy= 0.159996
 Thermal correction to Gibbs Free Energy= 0.105272
 Sum of electronic and zero-point Energies= -806.438943
 Sum of electronic and thermal Energies= -806.425715
 Sum of electronic and thermal Enthalpies= -806.424771
 Sum of electronic and thermal Free Energies= -806.479495

TS5OOH₂ (neutral radical)

C1 0.275460 -0.601439 -0.336488
 C2 -0.073295 0.730507 0.309591
 C3 -1.014063 1.389014 -0.723618
 C4 -1.871829 -0.734921 -0.629922
 C5 2.214531 0.397952 0.298426
 H6 1.359793 2.231739 0.818734
 O7 -0.844499 2.453977 -1.254854
 O8 3.397476 0.583056 0.414471
 N9 1.182001 1.254688 0.642875
 N10 1.614865 -0.759344 -0.253582
 N11 -0.610113 -1.318318 -0.917900
 N12 -2.124255 0.550064 -0.810704
 N13 -2.706524 -1.457675 0.140799
 H14 -2.193297 -1.000037 1.273309
 H15 -2.367538 -2.422597 0.151657
 O16 -0.993278 0.612673 1.461024
 O17 -1.226986 -0.658558 1.897693
 C18 2.365535 -1.877008 -0.791068
 H19 2.195101 -1.960809 -1.866715
 H20 2.053847 -2.801150 -0.300600
 H21 3.420516 -1.686861 -0.595000

Zero-point correction= 0.140143 (Hartree/Particle)
 Thermal correction to Energy= 0.151968
 Thermal correction to Enthalpy= 0.152912
 Thermal correction to Gibbs Free Energy= 0.101924
 Sum of electronic and zero-point Energies= -806.350416
 Sum of electronic and thermal Energies= -806.338591
 Sum of electronic and thermal Enthalpies= -806.337647
 Sum of electronic and thermal Free Energies= -806.388635

[5-OOH_{N2}-9MOG – H][•]

C1 -0.282781 0.691312 0.006741
 C2 -0.018234 -0.799808 0.097893
 C3 1.227722 -1.124571 -0.731346
 C4 1.924264 1.092081 -0.342907
 C5 -2.267237 -0.385700 -0.183587
 H6 -1.467456 -2.313346 -0.321868
 O7 1.336061 -2.167643 -1.340106
 O8 -3.455292 -0.554326 -0.281299
 N9 -1.260089 -1.325957 -0.325829
 N10 -1.627216 0.855724 0.044882
 N11 0.612497 1.588624 -0.158197
 N12 2.239577 -0.173695 -0.685547
 N13 2.947626 1.923296 -0.243557
 H14 1.909777 -1.317753 2.111559
 H15 2.573032 2.846269 -0.002361
 O16 0.143741 -1.224061 1.464414
 O17 1.286935 -0.581245 2.022917
 C18 -2.318870 2.128102 -0.020008
 H19 -2.133057 2.615804 -0.980539
 H20 -1.965666 2.772203 0.786261
 H21 -3.384136 1.930587 0.096566

Zero-point correction= 0.143739 (Hartree/Particle)
 Thermal correction to Energy= 0.156901
 Thermal correction to Enthalpy= 0.157845
 Thermal correction to Gibbs Free Energy= 0.103455
 Sum of electronic and zero-point Energies= -806.392230
 Sum of electronic and thermal Energies= -806.379068
 Sum of electronic and thermal Enthalpies= -806.378124
 Sum of electronic and thermal Free Energies= -806.432513

syn-TS5 (neutral radical)

C1 -0.072654 0.735833 -0.146091
 C2 0.033606 -0.704944 -0.286925
 C3 1.367736 -1.273017 -0.601571
 C4 2.156000 0.847254 -0.048744
 C5 -2.141260 -0.117661 -0.500231
 H6 -1.445065 -2.110009 -0.798716
 O7 1.472754 -2.418655 -1.007913
 O8 -3.330747 -0.192424 -0.661657
 N9 -1.195405 -1.149044 -0.614256
 N10 -1.397309 1.040543 -0.204263
 N11 0.932217 1.529007 0.012324
 N12 2.402623 -0.411323 -0.357084
 N13 3.201854 1.641478 0.225027
 H14 4.129883 1.252121 0.191823
 H15 3.050609 2.612516 0.439689
 O16 0.062450 -1.014444 1.710326
 O17 -1.094301 -1.302710 2.033047
 C18 -1.981462 2.358398 -0.051667
 H19 -1.577631 3.035882 -0.806788
 H20 -1.759916 2.749476 0.943092
 H21 -3.058791 2.256076 -0.180398

Zero-point correction= 0.144147 (Hartree/Particle)
 Thermal correction to Energy= 0.157420
 Thermal correction to Enthalpy= 0.158364
 Thermal correction to Gibbs Free Energy= 0.103499

Sum of electronic and zero-point Energies= -806.430372
 Sum of electronic and thermal Energies= -806.417099
 Sum of electronic and thermal Enthalpies= -806.416155
 Sum of electronic and thermal Free Energies= -806.471019

syn-[5-OO-9MOG – H][•]

C1 -0.119789 0.705318 -0.032972
 C2 0.014140 -0.793246 0.061365
 C3 1.304871 -1.256256 -0.632001
 C4 2.112427 0.847059 -0.111511
 C5 -2.161148 -0.211624 -0.401081
 H6 -1.490856 -2.201418 -0.509590
 O7 1.334174 -2.337414 -1.181952
 O8 -3.341230 -0.266939 -0.627304
 N9 -1.237897 -1.234043 -0.381058
 N10 -1.427896 0.987221 -0.163241
 N11 0.878532 1.512918 -0.024569
 N12 2.350682 -0.391256 -0.492771
 N13 3.153050 1.642193 0.158306
 H14 4.085230 1.268438 0.080587
 H15 2.997675 2.610665 0.383399
 O16 0.264800 -1.140607 1.499777
 O17 -0.757495 -0.857021 2.251616
 C18 -2.007371 2.311777 -0.266279
 H19 -1.557161 2.852385 -1.101920
 H20 -1.833704 2.861611 0.660359
 H21 -3.077233 2.186785 -0.431745

Zero-point correction= 0.146000 (Hartree/Particle)
 Thermal correction to Energy= 0.159120
 Thermal correction to Enthalpy= 0.160064
 Thermal correction to Gibbs Free Energy= 0.105692
 Sum of electronic and zero-point Energies= -806.440104
 Sum of electronic and thermal Energies= -806.426985
 Sum of electronic and thermal Enthalpies= -806.426041
 Sum of electronic and thermal Free Energies= -806.480413

TS5OOH_{N7} (neutral radical)

C1 -0.119384 0.709313 -0.179352
 C2 0.006794 -0.776701 -0.254963
 C3 1.412891 -1.271130 -0.592312
 C4 2.102474 0.897130 -0.065266
 C5 -2.107178 -0.267792 -0.537956
 H6 -1.516397 -1.456574 2.364211
 O7 1.593820 -2.394223 -1.001376
 O8 -3.298840 -0.385085 -0.653255
 N9 -1.150098 -1.318802 -0.631557
 N10 -1.440143 0.959308 -0.294279
 N11 0.849877 1.540772 -0.068195
 N12 2.399553 -0.348115 -0.353908
 N13 3.102297 1.735367 0.239684
 H14 4.046447 1.384795 0.247349
 H15 2.904743 2.704390 0.424285
 O16 0.099873 -1.223463 1.500794
 O17 -0.931553 -0.696456 2.207264
 C18 -2.083490 2.253810 -0.219960
 H19 -1.680007 2.915167 -0.989832

H20 -1.913620 2.697577 0.763367
H21 -3.150606 2.100973 -0.380162

Zero-point correction= 0.142787 (Hartree/Particle)
Thermal correction to Energy= 0.156191
Thermal correction to Enthalpy= 0.157136
Thermal correction to Gibbs Free Energy= 0.101943
Sum of electronic and zero-point Energies= -806.374889
Sum of electronic and thermal Energies= -806.361484
Sum of electronic and thermal Enthalpies= -806.360540
Sum of electronic and thermal Free Energies= -806.415733

[5-OOH_{N7}-9MOG - H][•]

C1 -0.149860 0.696424 0.105973
C2 -0.048315 -0.819250 0.110223
C3 1.146256 -1.129239 -0.948573
C4 2.056081 0.835998 -0.112302
C5 -2.172847 -0.200215 -0.334414
H6 -0.874318 -1.797358 2.468960
O7 1.047628 -2.037076 -1.726678
O8 -3.332064 -0.223858 -0.663570
N9 -1.339887 -1.306804 -0.121814
N10 -1.447725 0.997752 -0.071256
N11 0.849828 1.501316 0.120388
N12 2.212951 -0.319256 -0.725784
N13 3.141318 1.531557 0.236134
H14 4.053260 1.141262 0.061553
H15 3.037635 2.445548 0.644415
O16 0.516820 -1.348711 1.288976
O17 -0.332190 -0.998579 2.384733
C18 -1.989744 2.329766 -0.255156
H19 -1.544885 2.797907 -1.136665
H20 -1.771754 2.935699 0.625786
H21 -3.066313 2.229871 -0.389916

Zero-point correction= 0.143735 (Hartree/Particle)
Thermal correction to Energy= 0.157120
Thermal correction to Enthalpy= 0.158064
Thermal correction to Gibbs Free Energy= 0.103101
Sum of electronic and zero-point Energies= -806.395731
Sum of electronic and thermal Energies= -806.382345
Sum of electronic and thermal Enthalpies= -806.381401
Sum of electronic and thermal Free Energies= -806.436365

TSOOH_{N7} (neutral radical)

C1 0.028905 0.877419 -0.070145
C2 0.028435 -0.560016 -0.399282
C3 -1.307126 -1.195721 -0.666860
C4 -2.207812 0.831892 0.051350
C5 2.116771 0.142418 -0.440647
H6 1.426227 -1.897074 0.207588
O7 -1.379528 -2.319493 -1.118460
O8 3.312591 0.127051 -0.510810
N9 1.240983 -0.976176 -0.689459
N10 1.328157 1.259599 -0.098906
N11 -1.016550 1.584510 0.154530
N12 -2.384128 -0.406911 -0.341439
N13 -3.283415 1.551572 0.397025

H14 -4.192522 1.119905 0.352124
H15 -3.176018 2.510459 0.682393
O16 0.134513 -1.524020 1.585919
O17 1.153189 -2.238350 1.318286
C18 1.846690 2.585293 0.173441
H19 1.599254 2.879035 1.195529
H20 1.417516 3.304586 -0.527047
H21 2.928922 2.545722 0.050543

Zero-point correction= 0.140250 (Hartree/Particle)
Thermal correction to Energy= 0.153378
Thermal correction to Enthalpy= 0.154322
Thermal correction to Gibbs Free Energy= 0.099714
Sum of electronic and zero-point Energies= -806.401947
Sum of electronic and thermal Energies= -806.388818
Sum of electronic and thermal Enthalpies= -806.387874
Sum of electronic and thermal Free Energies= -806.442482

[9MOG - H - H_{N7}] + HOO[•]

C1 -0.033571 0.960084 -0.079433
C2 0.038428 -0.422386 -0.610935
C3 -1.260595 -1.173387 -0.745359
C4 -2.260036 0.760655 0.091786
C5 2.070666 0.350642 -0.524622
H6 1.384566 -2.316571 0.272998
O7 -1.269582 -2.313277 -1.160936
O8 3.263575 0.390972 -0.610704
N9 1.237494 -0.781280 -0.879241
N10 1.245593 1.396170 -0.056523
N11 -1.108394 1.563325 0.270012
N12 -2.372328 -0.463044 -0.368858
N13 -3.372146 1.405424 0.462819
H14 -4.257459 0.929345 0.393247
H15 -3.311451 2.340513 0.829984
O16 0.435080 -1.792808 1.769932
O17 1.271057 -2.628585 1.209167
C18 1.718957 2.683037 0.412919
H19 1.511407 2.793251 1.479369
H20 1.222967 3.483745 -0.139038
H21 2.794288 2.723264 0.240168

Zero-point correction= 0.143289 (Hartree/Particle)
Thermal correction to Energy= 0.157768
Thermal correction to Enthalpy= 0.158712
Thermal correction to Gibbs Free Energy= 0.099722
Sum of electronic and zero-point Energies= -806.406824
Sum of electronic and thermal Energies= -806.392346
Sum of electronic and thermal Enthalpies= -806.391402
Sum of electronic and thermal Free Energies= -806.450392

TS4OOH_{N7} (neutral radical)

C1 0.149331 -0.459875 -0.149874
C2 -0.035076 1.017991 -0.228201
C3 -1.454770 1.498754 -0.097624
C4 -2.090584 -0.762809 -0.352796
C5 2.080586 0.624271 -0.527046
H6 1.487149 -0.974919 2.526579
O7 -1.724951 2.665486 0.067760

O8 3.248890 0.826107 -0.705546
 N9 1.054898 1.646000 -0.413329
 N10 1.475092 -0.638985 -0.435697
 N11 -0.821385 -1.309320 -0.532987
 N12 -2.416022 0.502729 -0.190787
 N13 -3.075353 -1.675081 -0.416698
 H14 -4.030883 -1.367830 -0.335156
 H15 -2.854348 -2.644046 -0.572188
 O16 1.059735 -0.161600 2.216614
 O17 -0.090977 -0.596124 1.620245
 C18 2.165849 -1.903302 -0.561487
 H19 2.089611 -2.479372 0.365315
 H20 3.214039 -1.685314 -0.767983
 H21 1.740233 -2.487060 -1.380492

Zero-point correction= 0.141498 (Hartree/Particle)
 Thermal correction to Energy= 0.155191
 Thermal correction to Enthalpy= 0.156135
 Thermal correction to Gibbs Free Energy= 0.100248
 Sum of electronic and zero-point Energies= -806.363003
 Sum of electronic and thermal Energies= -806.349311
 Sum of electronic and thermal Enthalpies= -806.348367
 Sum of electronic and thermal Free Energies= -806.404254

[4-OOH_{N7}-9MOG - H]^{*}

C1 0.208879 -0.478396 0.184411
 C2 -0.028915 0.998992 -0.172047
 C3 -1.465401 1.450726 -0.074979
 C4 -2.006122 -0.819563 -0.471720
 C5 2.058446 0.599987 -0.661746
 H6 1.424991 -0.265353 2.589970
 O7 -1.769967 2.583801 0.205371
 O8 3.175143 0.817294 -1.047740
 N9 0.980435 1.582825 -0.651517
 N10 1.573244 -0.600263 -0.174847
 N11 -0.707398 -1.248131 -0.578512
 N12 -2.377869 0.446249 -0.355627
 N13 -2.951848 -1.754015 -0.641447
 H14 -3.914856 -1.463342 -0.702015
 H15 -2.691467 -2.706404 -0.836865
 O16 0.599770 0.185884 2.359292
 O17 -0.060945 -0.779946 1.550423
 C18 2.313700 -1.843112 -0.177161
 H19 2.262431 -2.319985 0.805490
 H20 3.352604 -1.609708 -0.412606
 H21 1.914826 -2.529921 -0.929636

Zero-point correction= 0.142858 (Hartree/Particle)
 Thermal correction to Energy= 0.156536
 Thermal correction to Enthalpy= 0.157480
 Thermal correction to Gibbs Free Energy= 0.101968
 Sum of electronic and zero-point Energies= -806.380256
 Sum of electronic and thermal Energies= -806.366578
 Sum of electronic and thermal Enthalpies= -806.365633
 Sum of electronic and thermal Free Energies= -806.421146

TS24 (neutral radical)

C1 0.297616 -0.484036 -0.204402

C2 0.198843 0.957536 -0.026342
 C3 -1.134545 1.600208 -0.261493
 C4 -1.891978 -0.655228 -0.162750
 C5 2.386273 0.383433 -0.023899
 H6 1.658844 2.408404 0.285576
 O7 -1.222473 2.821135 -0.251564
 O8 3.572824 0.519437 0.077714
 N9 1.414935 1.443110 0.102853
 N10 1.654422 -0.759981 -0.291022
 N11 -0.710469 -1.140814 -0.813831
 N12 -3.029550 -1.427146 -0.385514
 H13 -3.875304 -0.949410 -0.105228
 H14 -2.956239 -2.360011 -0.002998
 O15 -0.193318 -0.347247 1.404066
 O16 -1.529152 -0.722731 1.324077
 C17 2.230584 -2.092276 -0.357995
 H18 2.096091 -2.612387 0.593601
 H19 3.293589 -1.986605 -0.572468
 H20 1.740721 -2.646527 -1.159265
 N21 -2.115266 0.702538 -0.505669

Zero-point correction= 0.143325 (Hartree/Particle)
 Thermal correction to Energy= 0.155232
 Thermal correction to Enthalpy= 0.156177
 Thermal correction to Gibbs Free Energy= 0.105303
 Sum of electronic and zero-point Energies= -806.332643
 Sum of electronic and thermal Energies= -806.320736
 Sum of electronic and thermal Enthalpies= -806.319792
 Sum of electronic and thermal Free Energies= -806.370665

[2,4-OO-9MOG - H]^{*}

C1 0.275917 -0.477437 0.134888
 C2 0.199127 1.011632 0.053431
 C3 -1.138547 1.676365 0.070079
 C4 -1.862090 -0.576996 -0.310519
 C5 2.381922 0.421760 -0.161808
 H6 1.616251 2.472888 -0.267843
 O7 -1.203802 2.871983 0.326304
 O8 3.553795 0.606336 -0.339159
 N9 1.388319 1.494091 -0.122940
 N10 1.673993 -0.727454 0.020551
 N11 -0.582333 -0.811331 -0.941521
 N12 -2.937710 -1.244951 -0.906203
 H13 -3.821052 -0.813628 -0.668831
 H14 -2.928900 -2.242260 -0.739717
 O15 -0.261393 -0.971617 1.350723
 O16 -1.660114 -1.135517 1.058368
 C17 2.248396 -2.060056 -0.057958
 H18 2.045679 -2.603648 0.866029
 H19 3.324009 -1.951195 -0.195023
 H20 1.818690 -2.593829 -0.908718
 N21 -2.129542 0.831157 -0.281954

Zero-point correction= 0.144534 (Hartree/Particle)
 Thermal correction to Energy= 0.156960
 Thermal correction to Enthalpy= 0.157904
 Thermal correction to Gibbs Free Energy= 0.105287
 Sum of electronic and zero-point Energies= -806.345052

Sum of electronic and thermal Energies= -806.332626
Sum of electronic and thermal Enthalpies= -806.331682
Sum of electronic and thermal Free Energies= -806.384299

TS25 (neutral radical)

C1 -0.311095 0.666371 -0.108337
C2 -0.078557 -0.745251 0.334926
C3 0.915530 -1.358987 -0.689057
C4 1.884771 0.681583 -0.179868
C5 -2.333112 -0.322295 0.147069
H6 -1.579094 -2.251300 0.426657
O7 0.669804 -2.389508 -1.283231
O8 -3.526936 -0.470269 0.106219
N9 -1.370128 -1.265388 0.478742
N10 -1.643850 0.879551 -0.149443
N11 0.684860 1.440150 -0.329047
N12 2.038376 -0.590604 -0.776424
N13 3.007348 1.442982 -0.226777
H14 3.885990 0.956770 -0.135555
H15 2.940601 2.367597 0.168795
O16 0.617039 -0.670412 1.597304
O17 1.800318 0.034828 1.368739
C18 -2.300696 2.122913 -0.502584
H19 -2.047747 2.401763 -1.527789
H20 -1.983866 2.914152 0.179569
H21 -3.374974 1.961073 -0.416173

Zero-point correction= 0.144277 (Hartree/Particle)
Thermal correction to Energy= 0.156258
Thermal correction to Enthalpy= 0.157202
Thermal correction to Gibbs Free Energy= 0.105917
Sum of electronic and zero-point Energies= -806.394169
Sum of electronic and thermal Energies= -806.382188
Sum of electronic and thermal Enthalpies= -806.381244
Sum of electronic and thermal Free Energies= -806.432530

[2,5-OO-9MOG - H]•

C1 0.312011 -0.660198 -0.128907
C2 0.080869 0.742569 0.349219
C3 -0.880996 1.381420 -0.671000
C4 -1.885726 -0.644432 -0.108576
C5 2.336612 0.311491 0.166646
H6 1.596112 2.231017 0.537162
O7 -0.636386 2.402456 -1.280597
O8 3.531058 0.459067 0.145488
N9 1.374494 1.246865 0.529504
N10 1.646310 -0.870696 -0.188340
N11 -0.692402 -1.420669 -0.346707
N12 -3.027875 -1.410964 -0.246855
H13 -3.887448 -0.909374 -0.072098
H14 -2.968607 -2.314261 0.201423
O15 -0.629407 0.606975 1.597615
O16 -1.846150 -0.096454 1.308499
C17 2.300750 -2.115042 -0.541690
H18 2.152982 -2.857841 0.245668
H19 3.363925 -1.906903 -0.660648
H20 1.884820 -2.491838 -1.477857

N21 -2.025646 0.623751 -0.795579

Zero-point correction= 0.145554 (Hartree/Particle)
Thermal correction to Energy= 0.157683
Thermal correction to Enthalpy= 0.158627
Thermal correction to Gibbs Free Energy= 0.107253
Sum of electronic and zero-point Energies= -806.394094
Sum of electronic and thermal Energies= -806.381965
Sum of electronic and thermal Enthalpies= -806.381021
Sum of electronic and thermal Free Energies= -806.432395

**Cartesian coordinates for the structures
in Table 1, optimized at ω B97XD/
6-311+G(d,p).**

9MOG⁺·1MC

C1 -1.102139 1.065126 -0.006382
 C2 -2.510025 0.748123 -0.006122
 H3 0.729900 0.085639 -0.002545
 C4 -0.811240 -1.356644 0.002696
 C5 -4.767295 0.703543 -0.004789
 N6 -0.317001 -0.077560 -0.002742
 N7 -3.608437 1.518813 -0.009287
 N8 -4.288234 -0.617455 0.000353
 N9 -2.138627 -1.655593 0.007207
 C10 -2.931623 -0.616728 0.001600
 N11 0.047619 -2.348122 0.003956
 H12 -0.331649 -3.284388 0.008505
 H13 1.083001 -2.188171 -0.001669
 O14 -0.639750 2.197800 -0.009168
 C15 3.201548 -0.736448 -0.004703
 N16 2.461606 0.401554 0.000198
 C17 3.055793 1.600381 0.007804
 C18 5.196057 0.570892 0.006240
 N19 4.591072 -0.645525 -0.002407
 H20 6.279950 0.565611 0.008179
 O21 2.687426 -1.865812 -0.011298
 N22 2.278889 2.687874 0.011411
 H23 1.265533 2.600428 0.005116
 H24 2.687178 3.607688 0.016305
 C25 4.480174 1.721205 0.012020
 H26 4.971567 2.684571 0.019059
 C27 5.357255 -1.893039 -0.010279
 H28 5.105312 -2.487313 0.868761
 H29 5.117247 -2.468914 -0.904852
 H30 6.419622 -1.651034 -0.000576
 C31 -5.152217 -1.790711 0.017678
 H32 -4.877092 -2.456181 -0.801224
 H33 -5.049140 -2.312627 0.970245
 H34 -6.177817 -1.445437 -0.108115
 O35 -5.905756 1.077721 -0.006746
 H36 -3.644914 2.530342 -0.014891

Zero-point correction= 0.282181 (Hartree/Particle)
 Thermal correction to Energy= 0.302207
 Thermal correction to Enthalpy= 0.303151
 Thermal correction to Gibbs Free Energy= 0.231754
 Sum of electronic and zero-point Energies= -1090.605830
 Sum of electronic and thermal Energies= -1090.585803
 Sum of electronic and thermal Enthalpies= -1090.584859
 Sum of electronic and thermal Free Energies= -1090.656256

9MOG⁺·1MC_precursor

C1 0.937679 1.105268 -0.315572
 C2 2.345679 0.793826 -0.366866
 H3 -0.889807 0.118935 -0.287105
 C4 0.653687 -1.316242 -0.391603
 C5 4.602112 0.756987 -0.392863

N6 0.156445 -0.039416 -0.336538
 N7 3.441101 1.567743 -0.357345
 N8 4.127169 -0.565114 -0.432332
 N9 1.981430 -1.610457 -0.428481
 C10 2.771063 -0.569206 -0.413389
 N11 -0.202777 -2.309728 -0.409868
 H12 0.178901 -3.244163 -0.447677
 H13 -1.237815 -2.153263 -0.378333
 O14 0.472519 2.235355 -0.257226
 C15 -3.357499 -0.711502 -0.203167
 N16 -2.619222 0.427272 -0.176579
 C17 -3.212290 1.621322 -0.064172
 C18 -5.348105 0.585099 0.007533
 N19 -4.744333 -0.626341 -0.109350
 H20 -6.429661 0.575156 0.077853
 O21 -2.844278 -1.836311 -0.308335
 N22 -2.437232 2.709974 -0.046785
 H23 -1.426243 2.627151 -0.122773
 H24 -2.845183 3.626397 0.033150
 C25 -4.633754 1.736026 0.035400
 H26 -5.123927 2.695371 0.130094
 C27 -5.509430 -1.873793 -0.148624
 H28 -5.351462 -2.375551 -1.104188
 H29 -5.179826 -2.534782 0.653404
 H30 -6.566298 -1.640167 -0.023663
 C31 4.994828 -1.735291 -0.456599
 H32 4.903935 -2.283159 0.482648
 H33 4.712987 -2.379134 -1.290343
 H34 6.017899 -1.383118 -0.583923
 O35 5.739578 1.134314 -0.390486
 H36 3.474178 2.578601 -0.319511
 O37 1.181896 -0.791495 2.793441
 O38 1.997838 0.075541 2.602711

Zero-point correction= 0.287059 (Hartree/Particle)
 Thermal correction to Energy= 0.311064
 Thermal correction to Enthalpy= 0.312008
 Thermal correction to Gibbs Free Energy= 0.229271
 Sum of electronic and zero-point Energies= -1240.882400
 Sum of electronic and thermal Energies= -1240.858395
 Sum of electronic and thermal Enthalpies= -1240.857451
 Sum of electronic and thermal Free Energies= -1240.940188

anti-TS5

C1 0.908365 1.045037 -0.091603
 C2 2.328392 0.705299 0.094620
 H3 -0.932590 0.088052 -0.149035
 C4 0.610967 -1.363286 -0.188102
 C5 4.541733 0.719326 -0.380190
 N6 0.117777 -0.079898 -0.142161
 N7 3.407190 1.499736 -0.096785
 N8 4.067247 -0.615788 -0.474134
 N9 1.937118 -1.664562 -0.327251
 C10 2.738139 -0.645105 -0.271452
 N11 -0.246050 -2.347352 -0.163293
 H12 0.127247 -3.284280 -0.228917
 H13 -1.280100 -2.182476 -0.081122

O14 0.479339 2.183190 -0.138312
 C15 -3.380520 -0.721383 -0.071924
 N16 -2.637175 0.412113 -0.143346
 C17 -3.226871 1.611476 -0.215086
 C18 -5.369774 0.589621 -0.153552
 N19 -4.768789 -0.626533 -0.076633
 H20 -6.453656 0.587851 -0.153042
 O21 -2.868444 -1.850103 -0.002708
 N22 -2.446578 2.694634 -0.276899
 H23 -1.434217 2.606964 -0.248330
 H24 -2.851945 3.614580 -0.324775
 C25 -4.650495 1.735649 -0.225698
 H26 -5.139081 2.698491 -0.287055
 C27 -5.539537 -1.868706 0.007320
 H28 -5.257361 -2.533306 -0.809546
 H29 -5.335288 -2.369341 0.954655
 H30 -6.599763 -1.627561 -0.062393
 C31 4.918796 -1.749391 -0.810120
 H32 4.892781 -2.480803 -0.001476
 H33 4.570491 -2.207992 -1.736730
 H34 5.931447 -1.368453 -0.938502
 O35 5.666993 1.092449 -0.531411
 H36 3.445974 2.502308 0.025848
 O37 1.580514 -0.515533 2.401168
 O38 2.269812 0.427281 1.993594

Zero-point correction= 0.287815 (Hartree/Particle)
 Thermal correction to Energy= 0.310028
 Thermal correction to Enthalpy= 0.310972
 Thermal correction to Gibbs Free Energy= 0.234797
 Sum of electronic and zero-point Energies= -1240.864045
 Sum of electronic and thermal Energies= -1240.841833
 Sum of electronic and thermal Enthalpies= -1240.840889
 Sum of electronic and thermal Free Energies= -1240.917064

***anti*-[5-OO-9MOG]⁺·1MC**

C1 0.911530 0.986661 0.031550
 C2 2.349830 0.642846 0.388169
 H3 -0.937749 0.064240 -0.144036
 C4 0.595802 -1.406081 -0.084487
 C5 4.483268 0.695288 -0.451329
 N6 0.111757 -0.117189 -0.098972
 N7 3.390408 1.457101 -0.063216
 N8 4.020914 -0.664609 -0.481941
 N9 1.917613 -1.713556 -0.245133
 C10 2.733101 -0.714625 -0.145588
 N11 -0.266158 -2.378976 -0.013332
 H12 0.096264 -3.321926 -0.058435
 H13 -1.300845 -2.198931 0.055061
 O14 0.518252 2.129046 -0.062996
 C15 -3.378504 -0.714914 -0.054824
 N16 -2.623580 0.407758 -0.163471
 C17 -3.199926 1.608316 -0.298045
 C18 -5.352519 0.607571 -0.237238
 N19 -4.764770 -0.608943 -0.092114
 H20 -6.436110 0.615077 -0.260028
 O21 -2.877545 -1.843587 0.076433

N22 -2.407988 2.681169 -0.387951
 H23 -1.399057 2.588105 -0.316749
 H24 -2.802960 3.602497 -0.478171
 C25 -4.621395 1.743369 -0.345516
 H26 -5.100039 2.706443 -0.459272
 C27 -5.548827 -1.839706 0.031034
 H28 -5.261823 -2.539308 -0.754295
 H29 -5.362502 -2.303516 1.000488
 H30 -6.605499 -1.591807 -0.063556
 C31 4.821177 -1.763186 -1.006549
 H32 4.868469 -2.561814 -0.265650
 H33 4.376083 -2.138833 -1.929668
 H34 5.819044 -1.371740 -1.201484
 O35 5.580378 1.057089 -0.753266
 H36 3.476786 2.440971 0.149852
 O37 1.613094 -0.251716 2.427480
 O38 2.435989 0.596421 1.885573

Zero-point correction= 0.289629 (Hartree/Particle)
 Thermal correction to Energy= 0.311689
 Thermal correction to Enthalpy= 0.312633
 Thermal correction to Gibbs Free Energy= 0.237204
 Sum of electronic and zero-point Energies= -1240.872090
 Sum of electronic and thermal Energies= -1240.850031
 Sum of electronic and thermal Enthalpies= -1240.849086
 Sum of electronic and thermal Free Energies= -1240.924516

TS500H_{N1}

C1 0.961259 0.929691 0.419670
 C2 2.474350 0.535960 0.645427
 H3 0.818796 -0.516171 1.856956
 C4 0.528339 -1.333611 -0.015359
 C5 4.470005 0.700218 -0.487606
 N6 0.194947 -0.187364 0.713058
 N7 3.513646 1.377079 0.254326
 N8 3.921673 -0.601444 -0.742585
 N9 1.811552 -1.613418 -0.450822
 C10 2.696846 -0.703249 -0.226741
 N11 -0.410298 -2.183332 -0.258500
 H12 -0.139793 -3.026688 -0.751979
 H13 -1.473546 -1.967902 -0.074751
 O14 0.635099 2.045774 0.137951
 C15 -3.403447 -0.659501 -0.130354
 N16 -2.641749 0.426009 -0.345423
 C17 -3.209076 1.621719 -0.477009
 C18 -5.370395 0.674777 -0.253141
 N19 -4.789626 -0.542784 -0.085344
 H20 -6.453112 0.698363 -0.210692
 O21 -2.919989 -1.803734 0.036405
 N22 -2.392605 2.675801 -0.636916
 H23 -1.395838 2.539639 -0.532740
 H24 -2.755157 3.612509 -0.692068
 C25 -4.628798 1.791764 -0.453337
 H26 -5.098524 2.758094 -0.578700
 C27 -5.581295 -1.751406 0.147016
 H28 -5.366520 -2.488275 -0.627495
 H29 -5.329956 -2.180445 1.117762

H30 -6.638425 -1.487898 0.122312
 C31 4.542454 -1.549218 -1.661346
 H32 4.582338 -2.531592 -1.190815
 H33 3.966574 -1.601795 -2.587324
 H34 5.549414 -1.187804 -1.866602
 O35 5.521032 1.096319 -0.890828
 H36 3.670025 2.310520 0.607146
 O37 1.735117 -0.600933 2.567186
 O38 2.619928 0.271667 2.053175

Zero-point correction= 0.281197 (Hartree/Particle)
 Thermal correction to Energy= 0.303324
 Thermal correction to Enthalpy= 0.304268
 Thermal correction to Gibbs Free Energy= 0.227312
 Sum of electronic and zero-point Energies= -1240.780973
 Sum of electronic and thermal Energies= -1240.758846
 Sum of electronic and thermal Enthalpies= -1240.757902
 Sum of electronic and thermal Free Energies= -1240.834858

50OH_{N1}-[5-OO-9MOG]⁺·1MC

C1 0.711394 0.825893 0.505193
 C2 2.181964 0.381196 0.670127
 H3 1.069565 -0.943165 3.014994
 C4 0.387000 -1.327449 -0.455354
 C5 4.245250 0.817409 -0.249021
 N6 -0.091983 -0.135786 -0.001294
 N7 3.176777 1.357099 0.450128
 N8 3.788294 -0.439859 -0.764432
 N9 1.690266 -1.517868 -0.851441
 C10 2.523941 -0.644862 -0.394503
 N11 -0.436364 -2.329349 -0.609283
 H12 -0.062941 -3.192858 -0.976673
 H13 -1.394932 -2.256155 -0.226268
 O14 0.381105 1.946265 0.853319
 C15 -3.198228 -0.625747 0.136938
 N16 -2.357200 0.433330 -0.042750
 C17 -2.767064 1.642976 -0.448864
 C18 -5.001321 0.812626 -0.503610
 N19 -4.559379 -0.392061 -0.060224
 H20 -6.069578 0.901628 -0.662495
 O21 -2.827660 -1.753988 0.458084
 N22 -1.886588 2.629309 -0.576861
 H23 -0.973600 2.529694 -0.125463
 H24 -2.212933 3.551281 -0.819005
 C25 -4.155750 1.846571 -0.726416
 H26 -4.521011 2.806264 -1.066310
 C27 -5.471366 -1.518814 0.162974
 H28 -5.273943 -2.307983 -0.563883
 H29 -5.322672 -1.917196 1.166319
 H30 -6.494577 -1.161344 0.053833
 C31 4.545070 -1.224895 -1.728354
 H32 4.664628 -2.242215 -1.353876
 H33 4.022730 -1.241640 -2.686835
 H34 5.519635 -0.750667 -1.840267
 O35 5.322834 1.294479 -0.453110
 H36 3.313409 2.142723 1.070959
 O37 1.523506 -1.232860 2.209799

O38 2.408232 -0.136584 1.981084

Zero-point correction= 0.289081 (Hartree/Particle)
 Thermal correction to Energy= 0.311557
 Thermal correction to Enthalpy= 0.312501
 Thermal correction to Gibbs Free Energy= 0.236309
 Sum of electronic and zero-point Energies= -1240.815158
 Sum of electronic and thermal Energies= -1240.792682
 Sum of electronic and thermal Enthalpies= -1240.791738
 Sum of electronic and thermal Free Energies= -1240.867930

syn-TS5

C1 -0.842630 -0.959195 -0.231534
 C2 -2.261639 -0.619778 -0.047833
 H3 1.011063 -0.028022 -0.162813
 C4 -0.505661 1.447906 -0.105340
 C5 -4.476777 -0.527700 -0.491900
 N6 -0.035237 0.156068 -0.154334
 N7 -3.350578 -1.359069 -0.337098
 N8 -3.973720 0.800501 -0.418787
 N9 -1.823213 1.784951 -0.210414
 C10 -2.643362 0.777005 -0.241691
 N11 0.370218 2.409676 0.014999
 H12 0.014620 3.355738 0.025448
 H13 1.401269 2.220097 0.084876
 O14 -0.421992 -2.090740 -0.377993
 C15 3.477551 0.731662 0.033519
 N16 2.720395 -0.379726 -0.149959
 C17 3.294674 -1.581172 -0.284434
 C18 5.448464 -0.605695 -0.060552
 N19 4.863175 0.612646 0.078443
 H20 6.531153 -0.624131 -0.013678
 O21 2.980539 1.861865 0.164098
 N22 2.501578 -2.642734 -0.457639
 H23 1.490626 -2.538682 -0.464307
 H24 2.894431 -3.564250 -0.554144
 C25 4.715430 -1.730221 -0.245036
 H26 5.191584 -2.695003 -0.354746
 C27 5.648397 1.831797 0.281080
 H28 5.421593 2.551480 -0.505898
 H29 5.402172 2.277060 1.245809
 H30 6.706773 1.574576 0.252279
 C31 -4.806316 1.983635 -0.592459
 H32 -4.735374 2.613400 0.295172
 H33 -4.476784 2.540007 -1.471138
 H34 -5.832127 1.642869 -0.728642
 O35 -5.608890 -0.854924 -0.681109
 H36 -3.417853 -2.367649 -0.311929
 O37 -3.314523 -1.007084 2.266270
 O38 -2.235165 -0.549509 1.881774

Zero-point correction= 0.287751 (Hartree/Particle)
 Thermal correction to Energy= 0.310134
 Thermal correction to Enthalpy= 0.311078
 Thermal correction to Gibbs Free Energy= 0.233766
 Sum of electronic and zero-point Energies= -1240.866997
 Sum of electronic and thermal Energies= -1240.844615
 Sum of electronic and thermal Enthalpies= -1240.843671
 Sum of electronic and thermal Free Energies= -1240.920983

syn-[5-OO-9MOG]⁺·1MC

C1 -0.841699 -0.963316 -0.035621
 C2 -2.281180 -0.623864 0.315027
 H3 1.016719 -0.041836 -0.123638
 C4 -0.511201 1.435457 -0.069158
 C5 -4.418997 -0.629268 -0.502552
 N6 -0.032207 0.143631 -0.077548
 N7 -3.330388 -1.414120 -0.150225
 N8 -3.931933 0.724814 -0.527179
 N9 -1.825569 1.751892 -0.243961
 C10 -2.649529 0.751975 -0.186339
 N11 0.357092 2.402441 0.032462
 H12 0.002231 3.348124 -0.014197
 H13 1.388330 2.214533 0.120624
 O14 -0.450617 -2.099207 -0.185840
 C15 3.460272 0.718404 0.028639
 N16 2.702256 -0.393979 -0.146169
 C17 3.275627 -1.592244 -0.311190
 C18 5.431164 -0.609966 -0.144239
 N19 4.846361 0.604179 0.029851
 H20 6.514859 -0.624612 -0.132448
 O21 2.961983 1.844560 0.188142
 N22 2.480958 -2.655245 -0.468594
 H23 1.471038 -2.558614 -0.423720
 H24 2.873383 -3.575077 -0.582283
 C25 4.697051 -1.735309 -0.320258
 H26 5.173332 -2.696668 -0.456311
 C27 5.633665 1.823752 0.223687
 H28 5.381892 2.551265 -0.548288
 H29 5.414342 2.256989 1.200264
 H30 6.691390 1.570273 0.160788
 C31 -4.731170 1.847686 -0.998020
 H32 -4.758966 2.619289 -0.228018
 H33 -4.297851 2.252104 -1.914379
 H34 -5.735458 1.471399 -1.189730
 O35 -5.526403 -0.965785 -0.792651
 H36 -3.441973 -2.393936 0.070284
 O37 -3.389616 -0.365226 2.336174
 O38 -2.213256 -0.549138 1.819268

Zero-point correction= 0.289636 (Hartree/Particle)
 Thermal correction to Energy= 0.311701
 Thermal correction to Enthalpy= 0.312646
 Thermal correction to Gibbs Free Energy= 0.236988
 Sum of electronic and zero-point Energies= -1240.872212
 Sum of electronic and thermal Energies= -1240.850147
 Sum of electronic and thermal Enthalpies= -1240.849203
 Sum of electronic and thermal Free Energies= -1240.924861

TSOOH_{N2}

C1 -0.824959 -1.400801 -0.013741
 C2 -2.286536 -1.165724 -0.041260
 H3 0.928022 -0.356945 -0.212969
 C4 -0.705046 1.002610 -0.538306
 C5 -4.555064 -1.256232 0.015058
 N6 -0.136934 -0.265051 -0.275540
 N7 -3.277490 -1.975982 0.159939

N8 -4.186547 0.033556 -0.300059
 N9 -2.096997 1.166191 -0.604428
 C10 -2.815506 0.138027 -0.344730
 N11 -0.006147 2.051842 -0.714982
 H12 -0.713370 3.273318 0.208736
 H13 1.020196 1.899436 -0.629987
 O14 -0.366795 -2.506643 0.228255
 C15 3.300084 0.559200 -0.210661
 N16 2.628735 -0.615092 -0.047880
 C17 3.292792 -1.748487 0.200421
 C18 5.364647 -0.589429 0.135426
 N19 4.692117 0.562346 -0.114000
 H20 6.443807 -0.509209 0.198115
 O21 2.721935 1.626084 -0.441373
 N22 2.586826 -2.875079 0.356001
 H23 1.573460 -2.857730 0.311175
 H24 3.050464 -3.746351 0.551604
 C25 4.717958 -1.769355 0.299003
 H26 5.261912 -2.682472 0.498789
 C27 5.381025 1.841611 -0.292949
 H28 5.174857 2.238382 -1.287697
 H29 5.028293 2.558238 0.449420
 H30 6.451851 1.680580 -0.172231
 C31 -5.128783 1.132860 -0.503971
 H32 -4.996062 1.544367 -1.504945
 H33 -6.134259 0.728565 -0.394609
 H34 -4.949176 1.905561 0.244619
 O35 -5.624184 -1.762698 0.155787
 H36 -3.218123 -2.967538 0.382488
 O37 -1.193209 3.689739 1.003831
 O38 -1.886558 2.734393 1.543299

Zero-point correction= 0.284703 (Hartree/Particle)
 Thermal correction to Energy= 0.307392
 Thermal correction to Enthalpy= 0.308336
 Thermal correction to Gibbs Free Energy= 0.229832
 Sum of electronic and zero-point Energies= -1240.786964
 Sum of electronic and thermal Energies= -1240.764275
 Sum of electronic and thermal Enthalpies= -1240.763331
 Sum of electronic and thermal Free Energies= -1240.841835

[9MOG - H₂]⁺·1MC + HOO[•]

C1 -0.818030 -1.402395 -0.009504
 C2 -2.281884 -1.170008 -0.040895
 H3 0.932165 -0.357951 -0.216001
 C4 -0.703328 1.000853 -0.544932
 C5 -4.552041 -1.261332 0.013043
 N6 -0.133441 -0.268364 -0.279084
 N7 -3.269054 -1.978870 0.166146
 N8 -4.185699 0.024815 -0.313146
 N9 -2.097830 1.158937 -0.617415
 C10 -2.814069 0.133321 -0.356221
 N11 -0.008475 2.049887 -0.718694
 H12 -0.765274 3.315633 0.223766
 H13 1.017889 1.899591 -0.634135
 O14 -0.361899 -2.507387 0.239950
 C15 3.301610 0.561619 -0.215181

N16 2.632162 -0.613629 -0.049451
 C17 3.298250 -1.744868 0.202941
 C18 5.368027 -0.582177 0.136380
 N19 4.693607 0.567566 -0.116725
 H20 6.446969 -0.499787 0.199999
 O21 2.721924 1.626495 -0.450015
 N22 2.594494 -2.872559 0.361677
 H23 1.581141 -2.857157 0.318862
 H24 3.059843 -3.741923 0.561640
 C25 4.723339 -1.762892 0.302439
 H26 5.268800 -2.674450 0.505203
 C27 5.380105 1.847875 -0.297613
 H28 5.173533 2.242503 -1.293116
 H29 5.025623 2.565085 0.443378
 H30 6.451181 1.689086 -0.176152
 C31 -5.128940 1.123222 -0.520122
 H32 -4.995351 1.532381 -1.521884
 H33 -6.134283 0.718661 -0.410742
 H34 -4.949754 1.897405 0.227092
 O35 -5.617761 -1.771888 0.158589
 H36 -3.207184 -2.968248 0.399349
 O37 -1.252772 3.715077 1.010666
 O38 -1.879977 2.725876 1.580509

Zero-point correction= 0.285666 (Hartree/Particle)
 Thermal correction to Energy= 0.309118
 Thermal correction to Enthalpy= 0.310063
 Thermal correction to Gibbs Free Energy= 0.229590
 Sum of electronic and zero-point Energies= -1240.786024
 Sum of electronic and thermal Energies= -1240.762571
 Sum of electronic and thermal Enthalpies= -1240.761627
 Sum of electronic and thermal Free Energies= -1240.842099

TS5OOH_{N2}

C1 0.865740 1.035829 -0.117149
 C2 2.298166 0.718010 -0.072319
 H3 -0.957751 0.050808 -0.107381
 C4 0.614259 -1.391849 -0.045647
 C5 4.506536 0.719727 -0.538850
 N6 0.101303 -0.109921 -0.105155
 N7 3.350074 1.506700 -0.281565
 N8 4.047412 -0.613306 -0.558821
 N9 1.937044 -1.678573 -0.198311
 C10 2.721772 -0.642181 -0.307559
 N11 -0.188319 -2.424895 0.174574
 H12 2.021645 -1.265965 2.653364
 H13 -1.202907 -2.213144 0.004307
 O14 0.425481 2.169316 -0.157383
 C15 -3.368969 -0.737862 -0.187342
 N16 -2.639371 0.408970 -0.133317
 C17 -3.246542 1.600627 -0.093923
 C18 -5.376506 0.550461 -0.156059
 N19 -4.760153 -0.658362 -0.199246
 H20 -6.460289 0.535491 -0.168704
 O21 -2.841254 -1.856603 -0.227185
 N22 -2.483248 2.697303 -0.048532
 H23 -1.470776 2.620830 -0.068034

H24 -2.902478 3.611734 -0.022876
 C25 -4.671605 1.706734 -0.101467
 H26 -5.171926 2.664878 -0.067611
 C27 -5.512102 -1.913221 -0.261043
 H28 -5.279670 -2.439731 -1.187561
 H29 -5.238047 -2.548943 0.581372
 H30 -6.576798 -1.684911 -0.221734
 C31 4.920389 -1.763206 -0.768690
 H32 4.438050 -2.455263 -1.458797
 H33 5.854085 -1.395418 -1.192523
 H34 5.115211 -2.261764 0.182233
 O35 5.619096 1.116232 -0.712269
 H36 3.372882 2.516384 -0.206513
 O37 1.497263 -0.461774 2.480701
 O38 2.349258 0.416727 1.945306

Zero-point correction= 0.283784 (Hartree/Particle)
 Thermal correction to Energy= 0.306670
 Thermal correction to Enthalpy= 0.307614
 Thermal correction to Gibbs Free Energy= 0.229022
 Sum of electronic and zero-point Energies= -1240.773842
 Sum of electronic and thermal Energies= -1240.750956
 Sum of electronic and thermal Enthalpies= -1240.750012
 Sum of electronic and thermal Free Energies= -1240.828604

[5-OOH_{N2}-9MOG]⁺

C1 0.961694 1.073571 0.087021
 C2 2.422752 0.686401 0.339839
 H3 -0.934672 0.187776 0.062264
 C4 0.518487 -1.297443 0.332711
 C5 4.401754 0.456035 -0.813591
 N6 0.104561 0.000665 0.133394
 N7 3.416559 1.344133 -0.416448
 N8 3.871109 -0.858454 -0.572097
 N9 1.784798 -1.723534 0.097445
 C10 2.650094 -0.766449 -0.055328
 N11 -0.397902 -2.132146 0.755397
 H12 2.300771 -0.252565 3.120981
 H13 -1.446755 -2.123461 0.397117
 O14 0.589282 2.209445 -0.106095
 C15 -3.350295 -0.764164 -0.104681
 N16 -2.626853 0.375528 -0.115786
 C17 -3.222257 1.565521 -0.273513
 C18 -5.338573 0.499366 -0.409916
 N19 -4.725700 -0.705274 -0.254851
 H20 -6.416059 0.473564 -0.522470
 O21 -2.830620 -1.894624 0.033830
 N22 -2.450197 2.655144 -0.287691
 H23 -1.438942 2.585605 -0.209347
 H24 -2.856132 3.568739 -0.407281
 C25 -4.638925 1.660139 -0.424846
 H26 -5.138576 2.610885 -0.551759
 C27 -5.479703 -1.962792 -0.229642
 H28 -5.122688 -2.623241 -1.020090
 H29 -5.341019 -2.456250 0.732893
 H30 -6.534651 -1.739110 -0.382948
 C31 4.517092 -2.072654 -1.052192

H32 4.020941 -2.427795 -1.957633
 H33 5.556385 -1.828130 -1.268501
 H34 4.459865 -2.837306 -0.277629
 O35 5.465289 0.683822 -1.308701
 H36 3.621768 2.327865 -0.306195
 O37 1.749809 0.271141 2.521009
 O38 2.749043 0.902190 1.714941

Zero-point correction= 0.285955 (Hartree/Particle)
 Thermal correction to Energy= 0.308408
 Thermal correction to Enthalpy= 0.309352
 Thermal correction to Gibbs Free Energy= 0.232853
 Sum of electronic and zero-point Energies= -1240.813769
 Sum of electronic and thermal Energies= -1240.791316
 Sum of electronic and thermal Enthalpies= -1240.790372
 Sum of electronic and thermal Free Energies= -1240.866871

TSOOH_{N7}

C1 -0.870265 -0.861012 -0.367730
 C2 -2.306098 -0.505961 -0.256216
 H3 0.997109 0.030273 -0.196112
 C4 -0.486137 1.523891 -0.028988
 C5 -4.486834 -0.331505 -0.453752
 N6 -0.045846 0.235932 -0.194920
 N7 -3.362120 -1.247125 -0.473740
 N8 -3.979854 0.989781 -0.309349
 N9 -1.804320 1.902035 -0.072584
 C10 -2.647579 0.927944 -0.192721
 N11 0.403892 2.456738 0.161129
 H12 0.061789 3.402627 0.265696
 H13 1.438183 2.246117 0.196725
 O14 -0.453241 -1.980989 -0.564467
 C15 3.471499 0.742023 0.065640
 N16 2.701011 -0.347413 -0.176932
 C17 3.260418 -1.551520 -0.353552
 C18 5.423542 -0.618879 -0.049386
 N19 4.853045 0.601603 0.130461
 H20 6.504711 -0.655837 0.016506
 O21 2.989009 1.875068 0.234947
 N22 2.456236 -2.591749 -0.587723
 H23 1.447619 -2.471554 -0.614902
 H24 2.837216 -3.514016 -0.719426
 C25 4.677920 -1.723105 -0.294434
 H26 5.142235 -2.689597 -0.435487
 C27 5.651946 1.799549 0.397360
 H28 5.483191 2.539417 -0.385887
 H29 5.363319 2.230772 1.356441
 H30 6.704599 1.519438 0.420135
 C31 -4.805527 2.189814 -0.285115
 H32 -5.838539 1.881676 -0.442252
 H33 -4.706646 2.683624 0.682688
 H34 -4.491003 2.866445 -1.080880
 O35 -5.634954 -0.632339 -0.537197
 H36 -3.388898 -2.011508 0.595115
 O37 -3.086056 -2.071948 1.735751
 O38 -2.240573 -1.140283 1.871042

Zero-point correction= 0.283484 (Hartree/Particle)
 Thermal correction to Energy= 0.304861
 Thermal correction to Enthalpy= 0.305805
 Thermal correction to Gibbs Free Energy= 0.232110
 Sum of electronic and zero-point Energies= -1240.836708
 Sum of electronic and thermal Energies= -1240.815330
 Sum of electronic and thermal Enthalpies= -1240.814386
 Sum of electronic and thermal Free Energies= -1240.888081

[9MOG - H_{N7}]⁺·IMC + HOO[•]

C1 -0.831590 -1.028280 -0.399423
 C2 -2.284028 -0.709554 -0.482094
 H3 0.991878 -0.061348 -0.218425
 C4 -0.532684 1.391657 -0.228849
 C5 -4.438603 -0.623107 -0.606379
 N6 -0.051059 0.108717 -0.288412
 N7 -3.275187 -1.496032 -0.601394
 N8 -4.000051 0.730699 -0.501793
 N9 -1.856271 1.730840 -0.315154
 C10 -2.668245 0.727835 -0.418815
 N11 0.331256 2.359142 -0.088642
 H12 -0.037132 3.299978 -0.054453
 H13 1.367992 2.182925 -0.020545
 O14 -0.366756 -2.144580 -0.431558
 C15 3.459941 0.742003 0.005596
 N16 2.722607 -0.389095 -0.120360
 C17 3.317725 -1.586872 -0.180643
 C18 5.453245 -0.564674 0.009924
 N19 4.846608 0.650142 0.070109
 H20 6.535496 -0.561652 0.068562
 O21 2.943663 1.870815 0.066235
 N22 2.544685 -2.669088 -0.303067
 H23 1.533093 -2.580064 -0.349205
 H24 2.953125 -3.587415 -0.356077
 C25 4.740496 -1.709841 -0.114670
 H26 5.232850 -2.671541 -0.162837
 C27 5.610092 1.891959 0.206193
 H28 5.371723 2.563463 -0.618996
 H29 5.355073 2.384714 1.145311
 H30 6.672860 1.652088 0.191984
 C31 -4.899010 1.875360 -0.480764
 H32 -5.673456 1.707725 0.268166
 H33 -4.315399 2.759619 -0.226477
 H34 -5.361562 2.002138 -1.460706
 O35 -5.574524 -0.968476 -0.680122
 H36 -3.509503 -0.869043 3.363764
 O37 -3.356727 -0.649808 2.424472
 O38 -2.085556 -0.337671 2.322281

Zero-point correction= 0.286364 (Hartree/Particle)
 Thermal correction to Energy= 0.310518
 Thermal correction to Enthalpy= 0.311462
 Thermal correction to Gibbs Free Energy= 0.229141
 Sum of electronic and zero-point Energies= -1240.840617
 Sum of electronic and thermal Energies= -1240.816464
 Sum of electronic and thermal Enthalpies= -1240.815520
 Sum of electronic and thermal Free Energies= -1240.897840

TS50OH_{N7}

C1 -0.825909 -1.019672 -0.166756
 C2 -2.289381 -0.700141 -0.020030
 H3 1.010194 -0.059520 -0.144852
 C4 -0.515015 1.400533 -0.146642
 C5 -4.414865 -0.643346 -0.523659
 N6 -0.037196 0.113973 -0.155527
 N7 -3.293693 -1.509682 -0.355550
 N8 -3.961200 0.718224 -0.525663
 N9 -1.833389 1.729864 -0.305888
 C10 -2.648862 0.725419 -0.294561
 N11 0.348385 2.370854 -0.030214
 H12 -0.014334 3.314057 -0.062337
 H13 1.381804 2.191706 0.067010
 O14 -0.376667 -2.137700 -0.247125
 C15 3.468771 0.735779 0.041265
 N16 2.727718 -0.389399 -0.116832
 C17 3.320131 -1.582911 -0.248608
 C18 5.460445 -0.567954 -0.074533
 N19 4.856367 0.641631 0.064169
 H20 6.543970 -0.566690 -0.047924
 O21 2.954513 1.859810 0.167495
 N22 2.543485 -2.659845 -0.394029
 H23 1.531117 -2.574723 -0.374102
 H24 2.949970 -3.575787 -0.487823
 C25 4.744055 -1.706507 -0.234791
 H26 5.234521 -2.664139 -0.344224
 C27 5.623988 1.875996 0.240270
 H28 5.367624 2.585066 -0.547203
 H29 5.391037 2.324780 1.206694
 H30 6.685839 1.637110 0.190257
 C31 -4.813132 1.869192 -0.782164
 H32 -4.775346 2.550165 0.069472
 H33 -4.473284 2.383675 -1.682609
 H34 -5.828474 1.499928 -0.922637
 O35 -5.554148 -0.977473 -0.659431
 H36 -3.896079 -0.932692 2.646023
 O37 -3.392366 -0.182711 2.281988
 O38 -2.284237 -0.754500 1.761106

Zero-point correction= 0.286447 (Hartree/Particle)
 Thermal correction to Energy= 0.308898
 Thermal correction to Enthalpy= 0.309842
 Thermal correction to Gibbs Free Energy= 0.232739
 Sum of electronic and zero-point Energies= -1240.812479
 Sum of electronic and thermal Energies= -1240.790029
 Sum of electronic and thermal Enthalpies= -1240.789084
 Sum of electronic and thermal Free Energies= -1240.866187

[5-OOH_{N7}-9MOG]⁺·1MC

C1 -0.841147 -0.982481 -0.030676
 C2 -2.289060 -0.635302 0.351250
 H3 1.011179 -0.051101 -0.123810
 C4 -0.512353 1.422899 -0.088270
 C5 -4.386450 -0.669836 -0.505961
 N6 -0.037161 0.134589 -0.088289

N7 -3.328683 -1.520085 -0.098647
 N8 -3.906003 0.671522 -0.619023
 N9 -1.825525 1.732278 -0.305432
 C10 -2.637354 0.730464 -0.213404
 N11 0.349135 2.393914 0.027944
 H12 -0.007024 3.338022 -0.035438
 H13 1.379060 2.208877 0.134972
 O14 -0.435631 -2.108337 -0.179530
 C15 3.454821 0.714893 0.043760
 N16 2.700701 -0.398154 -0.140967
 C17 3.277748 -1.592993 -0.318897
 C18 5.430330 -0.604733 -0.145544
 N19 4.841439 0.605596 0.042178
 H20 6.514093 -0.615477 -0.135823
 O21 2.953207 1.838122 0.214794
 N22 2.486958 -2.656951 -0.485479
 H23 1.476754 -2.565086 -0.433818
 H24 2.882047 -3.574587 -0.607579
 C25 4.700008 -1.730682 -0.331968
 H26 5.179354 -2.688981 -0.478499
 C27 5.624670 1.825931 0.246141
 H28 5.371937 2.558495 -0.520784
 H29 5.402663 2.251409 1.225509
 H30 6.683277 1.576166 0.182905
 C31 -4.690375 1.770966 -1.161797
 H32 -4.885702 2.502365 -0.375546
 H33 -4.138210 2.243071 -1.975939
 H34 -5.629598 1.358068 -1.527765
 O35 -5.504659 -1.018365 -0.757371
 H36 -3.773564 -0.839117 2.788413
 O37 -3.447510 -0.089145 2.266663
 O38 -2.217573 -0.614252 1.766620

Zero-point correction= 0.287823 (Hartree/Particle)
 Thermal correction to Energy= 0.310386
 Thermal correction to Enthalpy= 0.311330
 Thermal correction to Gibbs Free Energy= 0.233607
 Sum of electronic and zero-point Energies= -1240.827766
 Sum of electronic and thermal Energies= -1240.805203
 Sum of electronic and thermal Enthalpies= -1240.804259
 Sum of electronic and thermal Free Energies= -1240.881982

TS24

C1 2.753525 -0.521588 0.099641
 C2 2.300075 0.890067 -0.077766
 C3 0.838510 1.196717 -0.122610
 C4 0.691901 -1.210681 -0.396713
 C5 4.575831 0.872036 -0.121236
 H6 3.304983 2.674587 -0.316011
 O7 0.443162 2.348500 -0.042248
 O8 5.657727 1.359941 -0.211263
 N9 3.319976 1.666035 -0.178660
 N10 4.160656 -0.420046 0.021855
 N11 2.030736 -1.227940 -0.874271

N12 -0.141761 -2.138647 -0.877751
 H13 -1.144553 -2.083298 -0.634329
 H14 0.256175 -3.041451 -1.088606
 O15 2.316461 -0.921226 1.416792
 O16 1.126974 -1.579064 1.202086
 C17 5.064473 -1.565446 0.095859
 H18 4.983392 -2.038951 1.075298
 H19 6.078729 -1.196203 -0.052271
 H20 4.810149 -2.275077 -0.692999
 N21 0.097131 0.077317 -0.248101
 H22 -0.969883 0.194397 -0.214394
 C23 -3.340037 -0.693130 -0.091307
 N24 -2.638615 0.474671 -0.087558
 C25 -3.265622 1.647716 0.043838
 C26 -5.364449 0.545034 0.176775
 N27 -4.727621 -0.646493 0.048395
 H28 -6.442647 0.501978 0.279563
 O29 -2.794399 -1.794976 -0.211986
 N30 -2.527378 2.764386 0.046355
 H31 -1.515385 2.718539 -0.015364
 H32 -2.963884 3.664465 0.154732
 C33 -4.686178 1.718563 0.178535
 H34 -5.202599 2.662797 0.284432
 C35 -5.452845 -1.917895 0.037644
 H36 -5.305000 -2.420253 -0.919237
 H37 -5.079071 -2.562924 0.833333
 H38 -6.512788 -1.717344 0.190988

Zero-point correction= 0.286345 (Hartree/Particle)
 Thermal correction to Energy= 0.307798
 Thermal correction to Enthalpy= 0.308743
 Thermal correction to Gibbs Free Energy= 0.234951
 Sum of electronic and zero-point Energies= -1240.768124
 Sum of electronic and thermal Energies= -1240.746672
 Sum of electronic and thermal Enthalpies= -1240.745727
 Sum of electronic and thermal Free Energies= -1240.819519

[2,4-OO-9MOG]⁺·1MC

C1 2.755263 -0.518341 0.032419
 C2 2.296505 0.916461 0.001842
 C3 0.825183 1.203371 -0.038341
 C4 0.701923 -1.243916 -0.365541
 C5 4.578772 0.894742 -0.006072
 H6 3.287362 2.713970 0.046787
 O7 0.424849 2.351842 0.077286
 O8 5.652725 1.403355 -0.008473
 N9 3.306391 1.694563 0.022588
 N10 4.165239 -0.401213 -0.045055
 N11 2.018563 -1.152865 -1.007373
 N12 -0.172450 -2.103725 -0.984629
 H13 -1.130430 -2.088636 -0.605098
 H14 0.203616 -3.031873 -1.125701
 O15 2.316369 -1.039407 1.282979
 O16 1.103682 -1.740247 0.961415
 C17 5.075079 -1.546421 -0.050912
 H18 5.000959 -2.082625 0.896267
 H19 6.086937 -1.164874 -0.183022

H20 4.817303 -2.202135 -0.883742
 N21 0.112244 0.083222 -0.236485
 H22 -0.955919 0.193439 -0.226151
 C23 -3.321532 -0.690345 0.012629
 N24 -2.629115 0.481015 -0.078541
 C25 -3.267874 1.654005 -0.064375
 C26 -5.362482 0.549587 0.112424
 N27 -4.714086 -0.641808 0.115973
 H28 -6.442789 0.506545 0.191019
 O29 -2.765891 -1.791685 0.010345
 N30 -2.536940 2.774657 -0.134062
 H31 -1.523542 2.731588 -0.107222
 H32 -2.982369 3.676086 -0.096331
 C33 -4.692277 1.724506 0.021313
 H34 -5.217632 2.669769 0.025181
 C35 -5.427759 -1.915813 0.211976
 H36 -5.248178 -2.508739 -0.685803
 H37 -5.069584 -2.473826 1.077581
 H38 -6.493333 -1.713493 0.316740

Zero-point correction= 0.287914 (Hartree/Particle)
 Thermal correction to Energy= 0.309625
 Thermal correction to Enthalpy= 0.310569
 Thermal correction to Gibbs Free Energy= 0.235611
 Sum of electronic and zero-point Energies= -1240.773151
 Sum of electronic and thermal Energies= -1240.751441
 Sum of electronic and thermal Enthalpies= -1240.750497
 Sum of electronic and thermal Free Energies= -1240.825455

[9MOG - H_{N1}]⁺·[1MC + H_{N3}]⁺

C1 -1.047606 0.940688 -0.015078
 C2 -2.474772 0.705247 -0.011404
 H3 1.442134 0.153457 -0.010072
 C4 -0.855830 -1.402619 -0.000551
 C5 -4.733933 0.763394 -0.003051
 N6 -0.278997 -0.181572 -0.010679
 N7 -3.540772 1.523799 -0.014365
 N8 -4.318918 -0.575216 0.006097
 N9 -2.199935 -1.695190 0.010246
 C10 -2.957705 -0.635277 0.003204
 N11 -0.056376 -2.464103 -0.000036
 H12 -0.477767 -3.379981 0.007662
 H13 0.956788 -2.358264 -0.011100
 O14 -0.583600 2.094817 -0.021182
 C15 3.275192 -0.783111 -0.009072
 N16 2.484277 0.348943 -0.003412
 C17 2.952316 1.621686 0.010433
 C18 5.150813 0.696040 0.020873
 N19 4.645307 -0.566438 0.006144
 H20 6.232099 0.771164 0.030316
 O21 2.800837 -1.905876 -0.025849
 N22 2.087622 2.614206 0.010697
 H23 1.058644 2.444764 -0.002095
 H24 2.427303 3.563676 0.020795
 C25 4.365893 1.802431 0.024097
 H26 4.799736 2.792339 0.037019
 C27 5.505482 -1.755702 -0.009060

H28 5.249589 -2.402561 0.830127
H29 5.359211 -2.304195 -0.940329
H30 6.542750 -1.434629 0.074101
C31 -5.232987 -1.706741 0.031169
H32 -4.990626 -2.388990 -0.784586
H33 -5.152135 -2.230418 0.985249
H34 -6.242657 -1.316641 -0.093687
O35 -5.856108 1.192079 -0.003182
H36 -3.530747 2.534890 -0.023892

Zero-point correction= 0.282552 (Hartree/Particle)
Thermal correction to Energy= 0.302535
Thermal correction to Enthalpy= 0.303479
Thermal correction to Gibbs Free Energy= 0.232200
Sum of electronic and zero-point Energies= -1090.605337
Sum of electronic and thermal Energies= -1090.585354
Sum of electronic and thermal Enthalpies= -1090.584410
Sum of electronic and thermal Free Energies= -1090.655689

[9MOG - H_{N1}]*[1MC + H_{N3}]⁺_precursor

C1 0.866976 0.994733 -0.282438
C2 2.293884 0.769015 -0.349102
H3 -1.614959 0.192069 -0.222634
C4 0.685786 -1.346303 -0.407998
C5 4.551198 0.841019 -0.401611
N6 0.104239 -0.130439 -0.318231
N7 3.354864 1.592843 -0.334246
N8 4.142845 -0.498254 -0.467638
N9 2.030465 -1.630036 -0.465959
C10 2.782866 -0.566891 -0.434446
N11 -0.109056 -2.410411 -0.445688
H12 0.315994 -3.322235 -0.510394
H13 -1.122034 -2.310606 -0.406281
O14 0.398587 2.143973 -0.196113
C15 -3.443202 -0.754261 -0.196036
N16 -2.656727 0.380191 -0.157344
C17 -3.128283 1.646520 -0.041895
C18 -5.320643 0.708044 0.013860
N19 -4.811886 -0.547702 -0.103842
H20 -6.400397 0.775444 0.080476
O21 -2.966530 -1.870952 -0.304123
N22 -2.268239 2.642752 -0.019079
H23 -1.239914 2.481082 -0.087628
H24 -2.611121 3.587345 0.065378
C25 -4.540286 1.817067 0.048700
H26 -4.976322 2.801434 0.144618
C27 -5.667045 -1.739679 -0.149217
H28 -5.548573 -2.241355 -1.110291
H29 -5.381349 -2.425837 0.648175
H30 -6.702501 -1.429287 -0.017453
C31 5.062647 -1.623186 -0.533562
H32 5.008673 -2.204137 0.388872
H33 4.803811 -2.256323 -1.383196
H34 6.066899 -1.219589 -0.659265
O35 5.671153 1.275487 -0.402647
H36 3.339721 2.601876 -0.271518
O37 1.343943 -0.924018 2.788881

O38 2.139490 -0.036860 2.604977

Zero-point correction= 0.287296 (Hartree/Particle)
Thermal correction to Energy= 0.311243
Thermal correction to Enthalpy= 0.312188
Thermal correction to Gibbs Free Energy= 0.229846
Sum of electronic and zero-point Energies= -1240.881871
Sum of electronic and thermal Energies= -1240.857923
Sum of electronic and thermal Enthalpies= -1240.856979
Sum of electronic and thermal Free Energies= -1240.939320

anti-TS5 (PT)

C1 0.855907 0.934160 -0.115875
C2 2.293987 0.677707 0.075670
H3 -1.627517 0.167514 -0.156582
C4 0.663993 -1.398363 -0.226479
C5 4.516213 0.793684 -0.346047
N6 0.086777 -0.174834 -0.184465
N7 3.341744 1.519655 -0.082409
N8 4.108921 -0.556345 -0.458578
N9 2.009644 -1.688413 -0.365779
C10 2.772078 -0.647056 -0.285701
N11 -0.129818 -2.454321 -0.206837
H12 0.289411 -3.370106 -0.261639
H13 -1.140101 -2.347717 -0.117822
O14 0.418908 2.091182 -0.148973
C15 -3.456460 -0.767160 -0.079206
N16 -2.667935 0.364716 -0.141370
C17 -3.136382 1.635723 -0.193883
C18 -5.332913 0.709289 -0.126587
N19 -4.826366 -0.551736 -0.073389
H20 -6.414230 0.783896 -0.116234
O21 -2.978453 -1.887798 -0.033277
N22 -2.271790 2.627935 -0.246867
H23 -1.245740 2.460815 -0.229682
H24 -2.610618 3.577081 -0.283010
C25 -4.549563 1.815525 -0.187948
H26 -4.985053 2.803896 -0.229988
C27 -5.685496 -1.739681 0.002196
H28 -5.441718 -2.418998 -0.814571
H29 -5.524787 -2.251160 0.951982
H30 -6.724123 -1.422364 -0.077906
C31 5.015830 -1.648883 -0.775934
H32 5.001699 -2.385317 0.028710
H33 4.712829 -2.120078 -1.712347
H34 6.014430 -1.225146 -0.877831
O35 5.627101 1.224303 -0.469604
H36 3.330406 2.521843 0.042623
O37 1.581670 -0.613722 2.376210
O38 2.233738 0.364730 1.992009

Zero-point correction= 0.288376 (Hartree/Particle)
Thermal correction to Energy= 0.310596
Thermal correction to Enthalpy= 0.311540
Thermal correction to Gibbs Free Energy= 0.235227
Sum of electronic and zero-point Energies= -1240.865198
Sum of electronic and thermal Energies= -1240.842979
Sum of electronic and thermal Enthalpies= -1240.842034
Sum of electronic and thermal Free Energies= -1240.918347

anti-[5-OO-9MOG – HN1][•]·[1MC + HN3]⁺

C1 0.859797 0.873336 0.013266
 C2 2.313968 0.611120 0.384733
 H3 -1.619337 0.149946 -0.142053
 C4 0.648444 -1.444685 -0.121864
 C5 4.457006 0.767135 -0.422677
 N6 0.081051 -0.215743 -0.125998
 N7 3.325184 1.474816 -0.049002
 N8 4.064660 -0.609111 -0.461601
 N9 1.989647 -1.737032 -0.292593
 C10 2.767531 -0.719489 -0.153371
 N11 -0.148071 -2.491169 -0.052769
 H12 0.262117 -3.412153 -0.097625
 H13 -1.158261 -2.372931 0.033814
 O14 0.459173 2.033891 -0.072803
 C15 -3.457664 -0.761853 -0.057123
 N16 -2.657481 0.359343 -0.151865
 C17 -3.111555 1.630061 -0.275429
 C18 -5.317308 0.726163 -0.223834
 N19 -4.824870 -0.535004 -0.095705
 H20 -6.397708 0.810441 -0.246886
 O21 -2.990359 -1.882863 0.052385
 N22 -2.235635 2.611990 -0.349763
 H23 -1.215709 2.438890 -0.283242
 H24 -2.562594 3.561942 -0.437569
 C25 -4.521990 1.821956 -0.317133
 H26 -4.947153 2.810663 -0.417333
 C27 -5.697289 -1.710982 0.011366
 H28 -5.456710 -2.418265 -0.782420
 H29 -5.547071 -2.194120 0.977451
 H30 -6.731866 -1.384989 -0.084194
 C31 4.915530 -1.664446 -0.989972
 H32 4.995283 -2.467685 -0.256566
 H33 4.493721 -2.053408 -1.918846
 H34 5.896417 -1.228219 -1.175778
 O35 5.540475 1.186566 -0.710085
 H36 3.358501 2.461762 0.160352
 O37 1.635194 -0.337628 2.425868
 O38 2.396786 0.565233 1.884410

Zero-point correction= 0.290472 (Hartree/Particle)
 Thermal correction to Energy= 0.312464
 Thermal correction to Enthalpy= 0.313408
 Thermal correction to Gibbs Free Energy= 0.238233
 Sum of electronic and zero-point Energies= -1240.873707
 Sum of electronic and thermal Energies= -1240.851716
 Sum of electronic and thermal Enthalpies= -1240.850772
 Sum of electronic and thermal Free Energies= -1240.925947

syn-TS5 (PT)

C1 -0.789038 -0.838536 -0.238903
 C2 -2.228927 -0.583241 -0.069233
 H3 1.712490 -0.113962 -0.154021
 C4 -0.557667 1.493658 -0.114451
 C5 -4.452129 -0.592213 -0.485254
 N6 -0.001965 0.261209 -0.169706
 N7 -3.286208 -1.370284 -0.347172

N8 -4.015241 0.753523 -0.412325
 N9 -1.893905 1.822657 -0.222658
 C10 -2.677228 0.791422 -0.247545
 N11 0.256805 2.527284 0.020639
 H12 -0.143954 3.452734 0.040922
 H13 1.265031 2.394106 0.095308
 O14 -0.362123 -1.989925 -0.378676
 C15 3.553957 0.778653 0.039377
 N16 2.748829 -0.329692 -0.135475
 C17 3.198266 -1.601086 -0.276063
 C18 5.406622 -0.724070 -0.072236
 N19 4.919265 0.537955 0.067120
 H20 6.485712 -0.819511 -0.036184
 O21 3.093515 1.900938 0.161261
 N22 2.320143 -2.570039 -0.432786
 H23 1.297360 -2.385302 -0.434709
 H24 2.644676 -3.519509 -0.533869
 C25 4.607470 -1.806911 -0.244366
 H26 5.027881 -2.796815 -0.352520
 C27 5.795591 1.700187 0.256793
 H28 5.610648 2.430953 -0.530781
 H29 5.594435 2.160617 1.224668
 H30 6.830515 1.364112 0.213944
 C31 -4.902745 1.895909 -0.568419
 H32 -4.859301 2.519388 0.325729
 H33 -4.604871 2.479233 -1.441218
 H34 -5.911900 1.508328 -0.704717
 O35 -5.570184 -0.977678 -0.664804
 H36 -3.305373 -2.380239 -0.323840
 O37 -3.279334 -1.022118 2.263518
 O38 -2.219681 -0.511849 1.888654

Zero-point correction= 0.288316 (Hartree/Particle)
 Thermal correction to Energy= 0.310657
 Thermal correction to Enthalpy= 0.311601
 Thermal correction to Gibbs Free Energy= 0.234573
 Sum of electronic and zero-point Energies= -1240.867849
 Sum of electronic and thermal Energies= -1240.845509
 Sum of electronic and thermal Enthalpies= -1240.844564
 Sum of electronic and thermal Free Energies= -1240.921593

syn-[5-OO-9MOG – HN1][•]·[1MC + HN3]⁺

C1 -0.793182 -0.845934 -0.034938
 C2 -2.252081 -0.587244 0.317210
 H3 1.698130 -0.130825 -0.111137
 C4 -0.564230 1.478353 -0.076802
 C5 -4.392640 -0.692061 -0.493183
 N6 -0.003589 0.245788 -0.087451
 N7 -3.269825 -1.425082 -0.141731
 N8 -3.972311 0.678576 -0.523253
 N9 -1.895148 1.784109 -0.274833
 C10 -2.684293 0.764676 -0.191579
 N11 0.239429 2.516911 0.046885
 H12 -0.160989 3.442242 0.004060
 H13 1.246335 2.388131 0.151750
 O14 -0.395448 -2.000795 -0.174396
 C15 3.540128 0.764512 0.038372

N16 2.734679 -0.345706 -0.121485
 C17 3.182984 -1.612142 -0.299104
 C18 5.392984 -0.726681 -0.170173
 N19 4.906313 0.530276 0.010536
 H20 6.473080 -0.817234 -0.179914
 O21 3.077735 1.882138 0.193143
 N22 2.302519 -2.583610 -0.433475
 H23 1.283092 -2.407206 -0.375021
 H24 2.625021 -3.530442 -0.562250
 C25 4.592616 -1.811254 -0.328626
 H26 5.013358 -2.797026 -0.468517
 C27 5.784388 1.694012 0.184082
 H28 5.574705 2.430146 -0.592228
 H29 5.608783 2.145859 1.160872
 H30 6.818674 1.361721 0.109338
 C31 -4.816547 1.760601 -1.004830
 H32 -4.882827 2.536579 -0.241265
 H33 -4.397688 2.179073 -1.921901
 H34 -5.802874 1.340411 -1.198579
 O35 -5.484845 -1.085001 -0.781360
 H36 -3.333980 -2.408579 0.077128
 O37 -3.378017 -0.373660 2.338329
 O38 -2.194182 -0.505521 1.821628

Zero-point correction= 0.290438 (Hartree/Particle)
 Thermal correction to Energy= 0.312457
 Thermal correction to Enthalpy= 0.313401
 Thermal correction to Gibbs Free Energy= 0.237969
 Sum of electronic and zero-point Energies= -1240.874062
 Sum of electronic and thermal Energies= -1240.852042
 Sum of electronic and thermal Enthalpies= -1240.851098
 Sum of electronic and thermal Free Energies= -1240.926530

TSOOH_{N2} (PT)

C1 -0.816061 -1.301235 -0.054015
 C2 -2.280172 -1.134155 -0.051004
 H3 1.636258 -0.423093 -0.148830
 C4 -0.772326 1.022307 -0.559771
 C5 -4.541467 -1.302869 0.049347
 N6 -0.137562 -0.181587 -0.304110
 N7 -3.251345 -1.975912 0.169575
 N8 -4.224810 0.001375 -0.270299
 N9 -2.172125 1.198189 -0.612532
 C10 -2.858202 0.149491 -0.339953
 N11 -0.109597 2.112347 -0.765848
 H12 -0.737536 3.235302 0.114089
 H13 0.902834 1.969371 -0.681705
 O14 -0.336204 -2.425014 0.181574
 C15 3.402358 0.615689 -0.200242
 N16 2.674806 -0.552875 -0.049869
 C17 3.206090 -1.775026 0.193991
 C18 5.347318 -0.725443 0.161558
 N19 4.780125 0.484767 -0.079487
 H20 6.428554 -0.732223 0.239039
 O21 2.868013 1.684127 -0.423053
 N22 2.395541 -2.807666 0.317983
 H23 1.364976 -2.705387 0.255738

H24 2.783972 -3.719959 0.501070
 C25 4.622538 -1.865213 0.302565
 H26 5.105908 -2.812585 0.494803
 C27 5.573537 1.710766 -0.229555
 H28 5.420153 2.129418 -1.224738
 H29 5.259637 2.442366 0.515275
 H30 6.624639 1.464340 -0.087218
 C31 -5.205769 1.064641 -0.461057
 H32 -5.092490 1.489893 -1.458872
 H33 -6.195776 0.623712 -0.351214
 H34 -5.053145 1.839717 0.291326
 O35 -5.599124 -1.836182 0.205945
 H36 -3.156111 -2.963746 0.387282
 O37 -1.177833 3.706199 0.935599
 O38 -1.885374 2.803205 1.530545

Zero-point correction= 0.284233 (Hartree/Particle)
 Thermal correction to Energy= 0.306780
 Thermal correction to Enthalpy= 0.307724
 Thermal correction to Gibbs Free Energy= 0.229519
 Sum of electronic and zero-point Energies= -1240.794071
 Sum of electronic and thermal Energies= -1240.771524
 Sum of electronic and thermal Enthalpies= -1240.770580
 Sum of electronic and thermal Free Energies= -1240.848785

[9MOG - H_{N1} - H_{N2}]·[1MC + H_{N3}]⁺ + HOO[•]

C1 -0.788245 -1.313338 -0.053811
 C2 -2.259377 -1.154589 -0.051978
 H3 1.656354 -0.420908 -0.161307
 C4 -0.764417 1.013739 -0.578683
 C5 -4.524375 -1.331408 0.045383
 N6 -0.123507 -0.198163 -0.327080
 N7 -3.217157 -1.994570 0.182323
 N8 -4.218304 -0.035732 -0.301065
 N9 -2.174582 1.170942 -0.646024
 C10 -2.850741 0.127210 -0.368570
 N11 -0.119374 2.105542 -0.757013
 H12 -0.936891 3.374275 0.162195
 H13 0.894246 1.970648 -0.679480
 O14 -0.311968 -2.435738 0.197065
 C15 3.415000 0.630060 -0.213731
 N16 2.694294 -0.542064 -0.053524
 C17 3.231978 -1.757302 0.209077
 C18 5.366465 -0.694060 0.175851
 N19 4.793131 0.509140 -0.083323
 H20 6.447237 -0.692803 0.259978
 O21 2.875157 1.691706 -0.452387
 N22 2.427777 -2.794195 0.342045
 H23 1.397085 -2.701071 0.275488
 H24 2.821858 -3.701047 0.539505
 C25 4.648197 -1.836899 0.326707
 H26 5.136547 -2.778619 0.533552
 C27 5.579049 1.738921 -0.241973
 H28 5.423956 2.148825 -1.240490
 H29 5.259697 2.474316 0.496839
 H30 6.631515 1.500134 -0.096733
 C31 -5.205404 1.022510 -0.496509

H32 -5.093647 1.442338 -1.496634
 H33 -6.193485 0.578108 -0.383996
 H34 -5.053950 1.801541 0.252108
 O35 -5.570118 -1.879207 0.215484
 H36 -3.111092 -2.976930 0.424174
 O37 -1.417842 3.794865 0.937383
 O38 -1.925751 2.799103 1.616187

Zero-point correction= 0.287250 (Hartree/Particle)
 Thermal correction to Energy= 0.310529
 Thermal correction to Enthalpy= 0.311473
 Thermal correction to Gibbs Free Energy= 0.231251
 Sum of electronic and zero-point Energies= -1240.791678
 Sum of electronic and thermal Energies= -1240.768399
 Sum of electronic and thermal Enthalpies= -1240.767455
 Sum of electronic and thermal Free Energies= -1240.847677

TS5OOH_{N2} (PT)

C1 0.846682 0.916501 -0.197003
 C2 2.288510 0.688841 -0.078987
 H3 -1.678568 0.166543 -0.219834
 C4 0.702822 -1.443252 -0.231724
 C5 4.523685 0.817606 -0.383454
 N6 0.106304 -0.222889 -0.252947
 N7 3.312088 1.535431 -0.188546
 N8 4.143909 -0.530289 -0.480817
 N9 2.059682 -1.702739 -0.336270
 C10 2.799001 -0.640694 -0.332541
 N11 -0.048299 -2.544608 -0.104123
 H12 2.078657 -1.434647 2.461399
 H13 -1.046240 -2.297880 -0.164433
 O14 0.378734 2.059244 -0.226032
 C15 -3.490312 -0.781235 -0.180998
 N16 -2.707104 0.361493 -0.173053
 C17 -3.179681 1.629398 -0.099160
 C18 -5.369766 0.687145 -0.031507
 N19 -4.861132 -0.569889 -0.106440
 H20 -6.450078 0.756625 0.024864
 O21 -3.005633 -1.893145 -0.248341
 N22 -2.320281 2.628772 -0.100272
 H23 -1.299318 2.464650 -0.155134
 H24 -2.661385 3.575920 -0.043772
 C25 -4.590708 1.799568 -0.024505
 H26 -5.029315 2.785344 0.038546
 C27 -5.713857 -1.765060 -0.122695
 H28 -5.592727 -2.289605 -1.071132
 H29 -5.425476 -2.430381 0.691175
 H30 -6.750057 -1.453988 0.001302
 C31 5.086685 -1.623668 -0.673515
 H32 4.667342 -2.331961 -1.388272
 H33 6.013245 -1.200676 -1.060120
 H34 5.278726 -2.127513 0.275560
 O35 5.623378 1.282066 -0.462756
 H36 3.276545 2.540528 -0.079168
 O37 1.468738 -0.678210 2.383428
 O38 2.210299 0.339942 1.931554

Zero-point correction= 0.285443 (Hartree/Particle)
 Thermal correction to Energy= 0.308127
 Thermal correction to Enthalpy= 0.309072
 Thermal correction to Gibbs Free Energy= 0.231477
 Sum of electronic and zero-point Energies= -1240.780006
 Sum of electronic and thermal Energies= -1240.757322
 Sum of electronic and thermal Enthalpies= -1240.756378
 Sum of electronic and thermal Free Energies= -1240.833973

[5-OOH_{N2}-9MOG - H_{N1}]*·[1MC + H_{N3}]⁺

C1 0.878849 0.909439 0.193821
 C2 2.386115 0.661135 0.337391
 H3 -1.636569 0.150728 0.056149
 C4 0.615143 -1.397357 0.417860
 C5 4.305889 0.556692 -0.928123
 N6 0.062584 -0.178102 0.276102
 N7 3.268480 1.374599 -0.507916
 N8 3.901015 -0.785590 -0.628123
 N9 1.893546 -1.770143 0.130321
 C10 2.700837 -0.773915 -0.051861
 N11 -0.189748 -2.362432 0.909998
 H12 -1.144392 -2.373343 0.514481
 H13 1.754581 0.839001 3.213396
 O14 0.458523 2.052274 0.049412
 C15 -3.436463 -0.817449 -0.143398
 N16 -2.666287 0.329669 -0.098940
 C17 -3.141002 1.591331 -0.224283
 C18 -5.310632 0.630630 -0.447923
 N19 -4.798187 -0.621636 -0.324569
 H20 -6.384128 0.689393 -0.586182
 O21 -2.949254 -1.927796 -0.031173
 N22 -2.287612 2.596954 -0.172361
 H23 -1.271207 2.443236 -0.071413
 H24 -2.626868 3.541721 -0.268305
 C25 -4.542917 1.750644 -0.406217
 H26 -4.984214 2.731544 -0.512651
 C27 -5.640310 -1.824296 -0.362394
 H28 -5.566646 -2.352694 0.588665
 H29 -6.670923 -1.521332 -0.540547
 H30 -5.302539 -2.482714 -1.162869
 C31 4.611818 -1.956986 -1.119467
 H32 4.603685 -2.724210 -0.345577
 H33 4.130977 -2.339480 -2.022257
 H34 5.633659 -1.653090 -1.343464
 O35 5.320059 0.860309 -1.486004
 H36 3.414534 2.370031 -0.413157
 O37 2.006520 0.161270 2.569951
 O38 2.814096 0.931291 1.674027

Zero-point correction= 0.287591 (Hartree/Particle)
 Thermal correction to Energy= 0.310194
 Thermal correction to Enthalpy= 0.311138
 Thermal correction to Gibbs Free Energy= 0.234537
 Sum of electronic and zero-point Energies= -1240.814359
 Sum of electronic and thermal Energies= -1240.791756
 Sum of electronic and thermal Enthalpies= -1240.790812
 Sum of electronic and thermal Free Energies= -1240.867414

TSOOH_{N7} (PT)

C1 -0.817724 -0.735885 -0.354156
 C2 -2.278116 -0.471620 -0.252267
 H3 1.698949 -0.069785 -0.178955
 C4 -0.547900 1.575021 -0.025152
 C5 -4.467096 -0.403599 -0.453889
 N6 -0.016751 0.348231 -0.188691
 N7 -3.298539 -1.261639 -0.475103
 N8 -4.030656 0.936871 -0.307300
 N9 -1.887909 1.941941 -0.071734
 C10 -2.691402 0.940812 -0.188360
 N11 0.277975 2.583683 0.183273
 H12 -0.111229 3.508383 0.291084
 H13 1.286920 2.432724 0.227756
 O14 -0.392990 -1.872232 -0.552824
 C15 3.545175 0.789744 0.077265
 N16 2.730315 -0.299368 -0.160625
 C17 3.167181 -1.568326 -0.356830
 C18 5.381854 -0.727298 -0.081427
 N19 4.906529 0.532753 0.111039
 H20 6.459195 -0.836737 -0.035448
 O21 3.094672 1.910496 0.246824
 N22 2.280848 -2.517627 -0.572889
 H23 1.262744 -2.317537 -0.585993
 H24 2.593698 -3.465553 -0.717044
 C25 4.573424 -1.791385 -0.315159
 H26 4.984501 -2.780040 -0.463269
 C27 5.793713 1.675161 0.362142
 H28 5.652935 2.427608 -0.414354
 H29 5.562393 2.115636 1.332340
 H30 6.823628 1.321628 0.352311
 C31 -4.913381 2.092995 -0.284411
 H32 -5.929873 1.732933 -0.439949
 H33 -4.839604 2.594078 0.682097
 H34 -4.634362 2.784341 -1.081023
 O35 -5.599763 -0.765115 -0.540987
 H36 -3.287970 -2.033483 0.578017
 O37 -2.990731 -2.097411 1.725779
 O38 -2.202310 -1.115968 1.878721

Zero-point correction= 0.284515 (Hartree/Particle)
 Thermal correction to Energy= 0.306694
 Thermal correction to Enthalpy= 0.307638
 Thermal correction to Gibbs Free Energy= 0.231266
 Sum of electronic and zero-point Energies= -1240.838056
 Sum of electronic and thermal Energies= -1240.815876
 Sum of electronic and thermal Enthalpies= -1240.814932
 Sum of electronic and thermal Free Energies= -1240.891305

[9MOG – H_{N1} – H_{N7}].[1MC + H_{N3}]⁺ + HOO[•]

C1 -0.759631 -0.904440 -0.389986
 C2 -2.232400 -0.676099 -0.482451
 H3 1.721654 -0.146107 -0.169575
 C4 -0.566904 1.435972 -0.239170
 C5 -4.390722 -0.689169 -0.619085
 N6 0.002310 0.214262 -0.276119
 N7 -3.188809 -1.507542 -0.601818

N8 -4.020252 0.679629 -0.523816
 N9 -1.911405 1.765221 -0.330602
 C10 -2.684614 0.738270 -0.431809
 N11 0.231642 2.479825 -0.105803
 H12 -0.182788 3.399315 -0.081767
 H13 1.242512 2.360550 -0.030849
 O14 -0.290441 -2.039214 -0.422672
 C15 3.544580 0.785486 0.014437
 N16 2.761062 -0.343729 -0.114799
 C17 3.235096 -1.613321 -0.178231
 C18 5.424384 -0.687556 0.019813
 N19 4.912793 0.571725 0.078197
 H20 6.504005 -0.761247 0.081294
 O21 3.064156 1.905357 0.069101
 N22 2.377673 -2.603928 -0.301353
 H23 1.352927 -2.432520 -0.349196
 H24 2.718367 -3.551870 -0.350914
 C25 4.647094 -1.791908 -0.105570
 H26 5.085393 -2.778877 -0.151243
 C27 5.765540 1.757971 0.219428
 H28 5.556469 2.456570 -0.590703
 H29 5.564108 2.247373 1.173109
 H30 6.807212 1.443342 0.176609
 C31 -4.967890 1.781414 -0.506904
 H32 -5.736626 1.583408 0.240771
 H33 -4.423693 2.690788 -0.252953
 H34 -5.434944 1.889520 -1.487193
 O35 -5.510355 -1.091220 -0.696260
 H36 -3.675926 -0.884305 3.322894
 O37 -3.475327 -0.626307 2.403285
 O38 -2.205653 -0.289107 2.384006

Zero-point correction= 0.286736 (Hartree/Particle)
 Thermal correction to Energy= 0.310980
 Thermal correction to Enthalpy= 0.311924
 Thermal correction to Gibbs Free Energy= 0.229184
 Sum of electronic and zero-point Energies= -1240.840169
 Sum of electronic and thermal Energies= -1240.815926
 Sum of electronic and thermal Enthalpies= -1240.814982
 Sum of electronic and thermal Free Energies= -1240.897722

TS5OOH_{N7} (PT)

C1 -0.769970 -0.894528 -0.169869
 C2 -2.254284 -0.664143 -0.025543
 H3 1.717564 -0.143248 -0.119538
 C4 -0.566455 1.447470 -0.152777
 C5 -4.385709 -0.704963 -0.518475
 N6 -0.001975 0.223152 -0.157154
 N7 -3.224392 -1.518896 -0.351368
 N8 -3.999936 0.670555 -0.522833
 N9 -1.904019 1.765807 -0.328030
 C10 -2.681830 0.738891 -0.299277
 N11 0.229829 2.492783 -0.022202
 H12 -0.179707 3.414302 -0.053706
 H13 1.237404 2.372176 0.085294
 O14 -0.315590 -2.030012 -0.252368
 C15 3.543637 0.781820 0.047662

N16 2.756914 -0.342747 -0.104023
 C17 3.228489 -1.606747 -0.243894
 C18 5.422770 -0.685652 -0.087112
 N19 4.913279 0.567833 0.053193
 H20 6.504031 -0.759674 -0.071122
 O21 3.064010 1.896588 0.168655
 N22 2.367177 -2.593444 -0.377135
 H23 1.342709 -2.426587 -0.354247
 H24 2.705969 -3.537829 -0.479684
 C25 4.641988 -1.784822 -0.236982
 H26 5.079124 -2.767306 -0.346270
 C27 5.769968 1.748342 0.217798
 H28 5.550440 2.472030 -0.567313
 H29 5.582976 2.208233 1.188813
 H30 6.810344 1.433870 0.150348
 C31 -4.903090 1.780653 -0.772179
 H32 -4.881743 2.468960 0.074348
 H33 -4.601688 2.305691 -1.680532
 H34 -5.904026 1.367956 -0.894571
 O35 -5.509251 -1.097498 -0.649524
 H36 -3.873755 -0.979276 2.626135
 O37 -3.396799 -0.202815 2.284251
 O38 -2.257478 -0.719077 1.768086

Zero-point correction= 0.287161 (Hartree/Particle)
 Thermal correction to Energy= 0.309553
 Thermal correction to Enthalpy= 0.310497
 Thermal correction to Gibbs Free Energy= 0.233686
 Sum of electronic and zero-point Energies= -1240.812878
 Sum of electronic and thermal Energies= -1240.790487
 Sum of electronic and thermal Enthalpies= -1240.789543
 Sum of electronic and thermal Free Energies= -1240.866353

[5-OOH_{N7}-9MOG - H_{N1}]^{*}·[1MC + H_{N3}]⁺

C1 -0.794808 -0.861303 -0.023977
 C2 -2.261119 -0.589410 0.379252
 H3 1.688064 -0.139979 -0.108420
 C4 -0.568733 1.468551 -0.096469
 C5 -4.349589 -0.743637 -0.498488
 N6 -0.012088 0.239734 -0.090466
 N7 -3.270606 -1.529781 -0.023817
 N8 -3.940237 0.613145 -0.626400
 N9 -1.897228 1.761689 -0.345516
 C10 -2.672634 0.741848 -0.214618
 N11 0.225673 2.512769 0.039172
 H12 -0.176673 3.435655 -0.027544
 H13 1.230390 2.389014 0.166890
 O14 -0.389958 -2.005964 -0.172586
 C15 3.527673 0.758106 0.047248
 N16 2.725140 -0.353119 -0.119797
 C17 3.176946 -1.617167 -0.307766
 C18 5.384793 -0.726201 -0.174943
 N19 4.894537 0.528125 0.015412
 H20 6.465135 -0.813398 -0.186917
 O21 3.062835 1.873477 0.211171
 N22 2.299985 -2.590215 -0.449004
 H23 1.280263 -2.416992 -0.387191

H24 2.624410 -3.535505 -0.584448
 C25 4.587471 -1.811761 -0.339966
 H26 5.010696 -2.795391 -0.487164
 C27 5.769276 1.693419 0.193799
 H28 5.558712 2.431656 -0.580331
 H29 5.591428 2.141776 1.171770
 H30 6.804552 1.364152 0.119183
 C31 -4.762059 1.660542 -1.210254
 H32 -4.982980 2.415442 -0.453505
 H33 -4.228003 2.121448 -2.043051
 H34 -5.686378 1.201874 -1.559156
 O35 -5.440200 -1.159655 -0.779681
 H36 -3.733055 -0.834954 2.789802
 O37 -3.417277 -0.057694 2.303926
 O38 -2.171163 -0.535057 1.793431

Zero-point correction= 0.288596 (Hartree/Particle)
 Thermal correction to Energy= 0.311084
 Thermal correction to Enthalpy= 0.312028
 Thermal correction to Gibbs Free Energy= 0.234720
 Sum of electronic and zero-point Energies= -1240.829285
 Sum of electronic and thermal Energies= -1240.806798
 Sum of electronic and thermal Enthalpies= -1240.805854
 Sum of electronic and thermal Free Energies= -1240.883162

TS24 (PT)

C1 2.782439 -0.528591 0.108980
 C2 2.286466 0.857266 -0.117445
 C3 0.817396 1.094670 -0.168782
 C4 0.741898 -1.243905 -0.410343
 C5 4.559584 0.916182 -0.139308
 H6 3.244890 2.661789 -0.405480
 O7 0.403496 2.262207 -0.078431
 O8 5.632694 1.429358 -0.236559
 N9 3.290551 1.661597 -0.231499
 N10 4.188211 -0.384886 0.043698
 N11 2.089660 -1.268714 -0.858377
 N12 -0.045499 -2.238156 -0.867407
 H13 -1.033698 -2.209161 -0.631127
 H14 0.380869 -3.144083 -0.988130
 O15 2.350078 -0.915022 1.435190
 O16 1.158259 -1.568556 1.238734
 C17 5.127362 -1.494455 0.156111
 H18 5.037909 -1.958654 1.139492
 H19 6.131738 -1.091614 0.028846
 H20 4.920155 -2.225198 -0.627711
 N21 0.084236 -0.008171 -0.286479
 H22 -1.647047 0.249771 -0.171839
 C23 -3.441934 -0.743770 -0.099805
 N24 -2.684288 0.413208 -0.074766
 C25 -3.177898 1.665271 0.072010
 C26 -5.343800 0.674406 0.187581
 N27 -4.812379 -0.567448 0.042684
 H28 -6.422016 0.716938 0.290828
 O29 -2.939656 -1.842869 -0.237657
 N30 -2.339362 2.683595 0.083391
 H31 -1.313153 2.556692 0.004231

H32 -2.701707 3.617896 0.195341
 C33 -4.588600 1.802855 0.206588
 H34 -5.044564 2.775439 0.326218
 C35 -5.639853 -1.779386 0.017177
 H36 -5.536281 -2.274533 -0.948966
 H37 -5.313888 -2.461306 0.802797
 H38 -6.678448 -1.495346 0.179982

Zero-point correction= 0.288911 (Hartree/Particle)
 Thermal correction to Energy= 0.310462
 Thermal correction to Enthalpy= 0.311406
 Thermal correction to Gibbs Free Energy= 0.236992
 Sum of electronic and zero-point Energies= -1240.779007
 Sum of electronic and thermal Energies= -1240.757456
 Sum of electronic and thermal Enthalpies= -1240.756512
 Sum of electronic and thermal Free Energies= -1240.830926

Zero-point correction= 0.287205 (Hartree/Particle)
 Thermal correction to Energy= 0.308584
 Thermal correction to Enthalpy= 0.309528
 Thermal correction to Gibbs Free Energy= 0.235952
 Sum of electronic and zero-point Energies= -1240.773356
 Sum of electronic and thermal Energies= -1240.751977
 Sum of electronic and thermal Enthalpies= -1240.751033
 Sum of electronic and thermal Free Energies= -1240.824609

[2,4-OO-9MOG - H_{N1}][•]·[1MC + H_{N3}]⁺

C1 2.799012 -0.526071 0.058581
 C2 2.289498 0.884465 -0.035879
 C3 0.812439 1.094532 -0.071486
 C4 0.764905 -1.295641 -0.293918
 C5 4.566689 0.948371 -0.086417
 H6 3.222829 2.712441 -0.116275
 O7 0.389188 2.261571 0.033473
 O8 5.627965 1.487325 -0.141494
 N9 3.278954 1.696648 -0.077486
 N10 4.204865 -0.363588 -0.040245
 N11 2.071319 -1.214488 -0.949343
 N12 -0.074541 -2.244691 -0.854674
 H13 -1.030080 -2.213450 -0.507661
 H14 0.316554 -3.177332 -0.868705
 O15 2.401720 -1.022304 1.334362
 O16 1.176089 -1.719067 1.069066
 C17 5.155018 -1.471267 -0.015374
 H18 5.098189 -1.986498 0.944701
 H19 6.152566 -1.055560 -0.153740
 H20 4.926277 -2.159812 -0.830358
 N21 0.110540 -0.013249 -0.236470
 H22 -1.655865 0.239619 -0.139808
 C23 -3.454953 -0.743898 -0.030766
 N24 -2.690027 0.410443 -0.057498
 C25 -3.180395 1.671645 0.001062
 C26 -5.356374 0.700051 0.100771
 N27 -4.829047 -0.550470 0.052917
 H28 -6.437204 0.754432 0.163566
 O29 -2.957551 -1.851139 -0.076476
 N30 -2.337701 2.685895 -0.014237
 H31 -1.307653 2.551501 -0.020900
 H32 -2.700809 3.625489 0.030929
 C33 -4.594020 1.823456 0.077845
 H34 -5.046425 2.803855 0.125060
 C35 -5.663865 -1.757384 0.069016
 H36 -5.547102 -2.297456 -0.871337
 H37 -5.355708 -2.403588 0.891028
 H38 -6.703123 -1.459772 0.200706