Table of Contents

Instrumentation and Experimental Methods

9-Methyl-8-oxoguanine (9MOG) was obtained from B. Lippert (University of Dortmund, Germany), which was prepared in W. Pfleiderer laboratory (University of Konstanz, Germany).[1] It may be synthesized from 8-bromo-9-methylguanine.[2] 2′-Deoxyguanosine (Sigma, > 99%), 8-oxo-2′-deoxyguanosine (OG, Sigma, ≥98%), $Cu(NO_3)_2$ (Alfa Aesar, 99.999%), KOH (Fisher Chemical, >85%) and H_2O_2 (Acros Organics, 35 wt%) were purchased from commercial sources and used as received. Chlorine gas (99.5%) was purchased from Sigma Aldrich. Helium gas (research grade) was purchased from T.W. Smith. All solvents were HPLC grade.

1. Generation and detection of $^1O_2$

$^1O_2$ was generated by the reaction of $H_2O_2 + Cl_2 + 2KOH \rightarrow {}^1O_2/{}^3O_2 + 2KCl + 2H_2O$.[3] 10.5 mL of 8 M KOH was added, at a flow rate of 0.5 mL/minute, to 20 mL of 35 wt% aqueous H_2O_2 which was immersed in a -17 ºC chiller. After completion of mixing, the mixture was immediately degassed. 3.42 sccm of Cl_2 was mixed with 53.5 sccm of He in a gas proportioner and bubbled through the H_2O_2/KOH slush. Cl_2 reacted completely with H_2O_2 and produced a mixture of $^1O_2$, $^3O_2$ and water. Gas products passed through a -70 ºC cold trap to remove water vapor. Only $^1O_2$, $^3O_2$ and He remained in the downstream gas. The concentration of $^1O_2$ was determined by measuring the $^1O_2$ phosphorescence $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ at 1270 nm [4] in an optical emission cell. Emission from the cell was collimated, passed through an optical chopper (Stanford Research Systems SR540) and filtered by a 5 nm-bandwidth interference filter centered at 1270 nm. The chopped emission was focused into a thermoelectrically cooled InGaAs photodetector (Newport 71887 detector and 77055 cooler) coupled with a lock-in amplifier (Stanford Research Systems SR830). The amplifier output was converted to absolute $^1O_2$ concentration following a calibration.[5] To reduce wall- and self-quenching of $^1O_2$, the sparger was continuously evacuated and its pressure was maintained at 12.8 τ using a Cole-Parmer 00244O pressure switch. At this pressure, a steady concentration of $^1O_2$ (~ 15%) was obtained.

2. Generation of $OG^{\bullet+}$ and $9MOG^{\bullet+}$ and ion-molecule scattering

Reactions of $^1O_2$ with $OG^{\bullet+}$ and $9MOG^{\bullet+}$ were carried out on a home-built ESI guided-ion-beam scattering tandem mass spectrometer.[6] The apparatus consists of an ESI ion source, a radio frequency (rf) hexapole ion guide, a quadrupole mass filter, an rf octopole ion guide running through a scattering cell, a second quadrupole mass filter and a pulse-counting electron multiplier ion detector.

A 3:1 methanol/water solution of 0.25 mM $Cu(NO_3)_2$ and 0.25 mM OG was freshly prepared and sprayed into the air through an ESI needle at a rate of 0.06 mL/hr. The Cu(II) complexes of nucleosides formed in the electrospray entered the source chamber of the mass spectrometer through a desolvation capillary which was biased at 156 V with respect to ground and heated up to 160 ºC. The source chamber was evacuated to a pressure of 1.6 τ. A skimmer with the orifice of 1.0 mm-diameter was located 3 mm away from the end of the desolvation capillary, separating the source chamber and the hexapole ion guide. The skimmer was biased at 23 V with respect to ground. The electrical field between the capillary and the skimmer prompted CID of Cu^{II}-OG complexes with the background gas in the source chamber. It is reasonable to assume the Cu^{II}-OG complexes have the similar complexation and dissociation properties as those of Cu^{II}-guanosine.[7] Accordingly, the formation of $OG^{\bullet+}$ in the experiment was due to the dissociation of $[Cu^{II}(OG)_3]^{\bullet 2+} \rightarrow [Cu^{I}(OG)_2]^+ + OG^{\bullet+}$. The intensity of the $OG^{\bullet+}$ ion beam could be increased by a factor of 2 – 3 with the addition of equimolar concentration of 2′-deoxyguanosine in the ESI solution, *i.e.*, 7×10^4 counts/sec (cps) of $OG^{\bullet+}$ in the presence of 0.25 mM 2′-deoxyguanosine *vs.* 3 ×

10^4 cps in the absence of the co-ligand. The relative formation efficiency of $[Cu^{II}(OG)_3]^{\bullet 2+}$, $[Cu^{II}(OG)_2G]^{\bullet 2+}$ and $[Cu^{II}OG(G)_2]^{\bullet 2+}$ were 1 : 2: 7 in our ESI ion source. Clearly, the Cu^{II}-complexes consisting of both ligand OG and co-ligand 2′-deoxyguanosine has a higher formation efficiency than $[Cu^{II}(OG)_3]^{\bullet 2+}$. Upon the dissociation of the complexes, formation of $OG^{\bullet +}$ was favored over $G^{\bullet +}$ as OG has a lower ionization energy. In view of the enhancement of $OG^{\bullet +}$ formation by 2′-deoxyguanosine, $9MOG^{\bullet +}$ was generated using an ESI solution of an equimolar concentration mixture of 9MOG, 2′-deoxyguanosine and $Cu(NO_3)_2$. The $9MOG^{\bullet +}$ ion beam intensity was 10×10^4 cps.

The $OG^{\bullet +}$ or $9MOG^{\bullet +}$ cations were transported into the hexapole ion guide for collisional focusing and thermalization to 310 K, followed by mass selection in the first quadrupole mass filter. By the combination of collisional damping in the hexapole and reducing the radius of the ion beam at the exit of the first quadrupole, the initial kinetic energy of the ion beam was reduced to 0.8 eV with an energy spread of < 0.7 eV. The mass-selected reactant radical ions were injected into the octopole ion guide that passes the scattering cell containing the $^1O_2$ reactant. In addition to generating an ion trapping potential in the radial direction, the octopole was biased at a DC potential. The DC offset was utilized to adjust the reactant ion kinetic energy in the laboratory frame (E_{lab}) and thereby control the E_{col} between radical cations and $^1O_2$ in the center-of-mass frame, *i.e.*, $E_{col} = E_{lab} \times m_{neutral}/(m_{ion} + m_{neutral})$ where $m_{neutral}$ and m_{ion} are the masses of $^1O_2$ and radical cations, respectively. The product ions resulting from reactive ion-molecule scattering and the remaining reactant ions were collected by the octopole, passed into the second quadrupole mass filter for mass analysis, and counted by the ion detector. Reaction cross sections were calculated from the ratio of reactant/product ion intensities at each E_{col}, the pressure and the concentration of $^1O_2$ in the scattering cell, and the effective cell length. The scattering cell gas pressure (including $^1O_2$, $^3O_2$ and He) was maintained at 0.2 mτ. At this pressure, $OG^{\bullet +}$ or $9MOG^{\bullet +}$ had at most single collisions with O_2 (including both ground- and excited state O_2).

Finally, we have conducted a control experiment under the same conditions except that pure ground-state O_2 was used as the collisional gas and confirmed that $OG^{\bullet +}$ and $9MOG^{\bullet +}$ are not reactive with $^3O_2$.

Computational Approaches

1. Molecular direct dynamics simulations

The initial trajectory conditions for the collisions of $9MOG^{\bullet +}$ with $^1O_2$ were set up by using the Venus program.[8] A 300 K quasi-classical Boltzmann distribution[9] was sampled for reactants vibrational energy (E_{vib}, including ZPE) and rotational energy (E_{rot}). Trajectories were started with a center-of-mass separation of 7.0 Å between randomly oriented $9MOG^{\bullet +}$ and $^1O_2$. Relative velocities were added to reactants corresponding to E_{col} = 0.05 eV at which the reaction efficiency was the highest in the experiment. The main purpose of the trajectory simulations was to probe the gross feature of collision dynamics and identify probable reaction pathway(s) and product structure(s). Therefore trajectories were calculated as head-on collisions, *i.e.*, the impact parameter for the collisions was set to zero. Hessian-based predictor-corrector algorithm[10] implemented in Gaussian 09[11] was used to integrate classical equations of motion, with Hessian recalculated every 5 steps. Trajectories were propagated with a step size of 0.25 $amu^{1/2}$Bohr (which corresponds to a step size of 0.6 fsec in the trajectory time). A quadratically convergent SCF procedure[12] was adopted in the trajectory integration in case the first-order SCF failed to converge. Trajectories were terminated when product separation exceeded 8.0 Å or a maximum trajectory integration time was reached. gOpenMol[13] was used for trajectory visualization. Sorting of reaction pathways and analysis of trajectory ensembles were carried out using custom programs written for these purposes.

A multi-reference level of theory was impractical for calculating a large batch of trajectories, as millions of Hessians are needed even for a single trajectory. Considering both computational cost and the usefulness of trajectory results, the ωB97XD/6-31G(d) level of theory was chosen for trajectory calculations. The ωB97XD method overestimated the $^1O_2$ excitation energy by 0.7 eV and consequently lowered most of the reaction energies. As such, the trajectories were likely not to miss reaction pathways that have happened in the experiment. In addition, the ωB97XD method has predicted similar reaction PES as the multi-reference methods, and the ωB97XD-calculated spin density distributions are consistent with the SOMOs mapped out at the multi-reference level of theory. Therefore, the ωB97XD trajectories sufficed the purpose for the identification of possible reaction pathways. A small batch of trajectories were recalculated at the ωB97XD/6-31+G(d,p) level of theory to test how a basis set with diffusion and *p* polarization would affect collision outcome. The two sets of the trajectory turned out to follow the same collision dynamics and produce the similar product recoil and internal energy distributions.

2. Reaction PES calculations

Structures of reaction intermediates, transition states (TSs) and products were evaluated first at the ωB97XD/6-31G+(d,p) level of theory. All TSs were verified by frequency analysis as first-order saddle points, and the vibrational mode associated with an imaginary frequency corresponds to the anticipated reaction pathway. Intrinsic reaction coordinate (IRC) calculation was carried out to substantiate the reactant/product minima connected through each TS.

Due to the mixed open- and closed-shell character of $^1O_2$,[14] a reaction system of doublet-state radical cation with $^1O_2$ presents multiconfigurational wavefunctions. The spin-restricted DFT was unable to describe the static correlation arising from the two degenerate π* orbitals of $^1O_2$ and overestimated the $^1O_2$ excitation energy, whereas the broken-symmetry, spin-unrestricted DFT brought in spin contamination from $^3O_2$. The problem exited not only in the $^1O_2$ reactant but also in its reaction intermediates and TSs with nucleobase.[15] To assess whether reaction structures are dominated by single-determinant wave functions, a T1 diagnostic[16] was performed at the CCSD(T)/aug-cc-pVTZ level of theory.

To obtain reliable energetics for reaction PES, we have evaluated the energies of the DFT optimized reaction structures using two multi-reference complete active space self-consistent field methods, CASSCF/6-31+G(d,p)[17] and CASPT2/6-31G(d,p)[18], the latter of which adds dynamic correlation using second order perturbation theory with the CASSCF wave function as the reference. The sizes of the active space are (9, 7) for 9MOG$^{\bullet+}$, (12, 8) for $^1O_2$, and (21, 15) for the reaction structures, so as to include the $\sigma_{O(2\sigma)-O(2\sigma)}$, $\sigma^*_{O(2\sigma)-O(2\sigma)}$, $\sigma_{O(2\pi)-O(2\pi)}$, $\pi_{\pm1}$, $\pi^*_{\pm1}$ and $\sigma^*_{O(2\pi)-O(2\pi)}$ orbitals in O_2, and the π and σ_{N-H} orbitals in 9MOG that have participated in the formation of $^1O_2$-adducts and hydroperoxides. Reaction enthalpy reported at each level of theory is based on the sum of the electronic energy calculated at the specified level and the 298 K thermal correction at ωB97XD/6-31+G(d,p) (including ZPE which was scaled by factor of 0.975[19]).

The ωB97XD/6-31+G(d,p) and CASSCF(21,15)/6-31+G(d,p) calculations were completed using Gaussian 09.[11] The DLPNO-CCSD(T)/aug-cc-pVTZ calculations and T1 diagnostic were calculated with ORCA 4.[20] The CASPT2(21,15)/6-31G(d,p) calculations were carried out using MOLCAS 8,[21] for which the shift parameter for ionization potential-electron affinity (IPEA) was set to 0.25 a.u.[22]

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Table S1. Relative enthalpies (eV, 298 K) calculated at the single- and multi-reference levels of theory and T1 diagnostics of wavefunctions

Species	ωB97XD/ 6-31+G(d,p)	DLPNO-CCSD(T)/ aug-cc-pVTZ [a]	CASSCF(21,15)/ 6-31+G(d,p) [a,b]	CASPT2(21,15)/ 6-31G(d,p) [a,c]	$<S^2>$		T1 diagnostic
					Before [d]	After [e]	
$9MOG^{\bullet+}$	0.0	0.0	0.0	0.0	0.763	0.750	0.017 ($9MOG^{\bullet+}$)
$^1O_2$					0.000	0.000	0.015 ($^1O_2$)
precursor	-1.75	-0.61	-1.37	-1.29	1.749	0.821	0.026
			2,4-addition				
TS24	1.14	1.40	3.00	2.16	0.800	0.750	0.026
$[2,4\text{-OO-}9MOG]^{\bullet+}$	0.88	0.86	1.75	1.63	0.757	0.750	0.016
			C4-addition				
TS-4OO	-0.07	0.03	1.66	0.47	0.755	0.750	0.020
$[4\text{-OO-}9MOG]^{\bullet+}$	-0.09	0.01	1.58	0.43	0.755	0.750	0.020
TS-PT1-4OO	1.84	2.13	4.40	2.73	0.771	0.750	0.029
$[4\text{-}OOH^1\text{-}9MOG]^{\bullet+}$	0.89	0.92	2.58	1.40	0.774	0.750	0.020
			C5-addition				
TS-*syn*-5OO	-1.30	-1.12	-0.85	-0.94	0.880	0.752	0.020
syn-$[5\text{-OO-}9MOG]^{\bullet+}$	-1.41	-1.23	-0.34	-0.84	0.754	0.750	0.019
TS-PT7-5OO	0.36	0.67	1.50	1.17	0.763	0.750	0.019
$[5\text{-}OOH^7\text{-}9MOG]^{\bullet+}$	-0.19	-0.17	0.89	0.51	0.763	0.750	0.016
TS-*rot*-5OO	-1.33	-1.14	-0.55	-0.73	0.754	0.750	0.019
TS-*anti*-5OO	-1.22	-1.02	-0.74	-0.87	0.946	0.753	0.019
anti-$[5\text{-OO-}9MOG]^{\bullet+}$	-1.41	-1.22	-0.58	-0.84	0.755	0.750	0.019
TS-PT1-5OO	0.39	0.51	3.05	1.03	0.755	0.750	0.017
$[5\text{-}OOH^1\text{-}9MOG]^{\bullet+}$	-0.36	-0.03	2.65	0.02	0.757	0.750	0.028
TS-PT2-5OO	1.43	1.62	4.69	1.84	0.763	0.750	0.026
$[5\text{-}OOH^2\text{-}9MOG]^{\bullet+}$	-0.04	0.01	1.40	0.60	0.770	0.750	0.017
			Hydrogen abstraction				
TS-OOH^2	0.51	0.68	2.25	1.10	1.019	0.758	0.019
$[9MOG - H^2]^+ + HOO^{\bullet}$	0.52	0.45	1.71	0.93	0.755	0.750	0.019
TS-PT2-4OO	1.14	1.12	2.62	1.81	0.866	0.755	0.021
$[4\text{-}OOH^2\text{-}9MOG]^{\bullet+}$	0.80	0.73	1.95	1.16	0.787	0.750	0.017
TS-OOH^7	-0.01	0.30	1.39	0.72	1.072	0.756	0.018
$[9MOG - H^7]^+ + HOO^{\bullet}$	-0.42	-0.40	0.67	0.25	0.756	0.750	0.019
TS-PT7-4OO	0.98	1.05	2.80	1.73	0.766	0.750	0.021
$[4\text{-}OOH^7\text{-}9MOG]^{\bullet+}$	0.68	0.74	1.28	1.40	0.762	0.750	0.018

[a] using ωB97XD/6-31+G(d,p)-calculated geometries and thermal corrections.
[b] CASSCF(9,7)/6-31+G(d,p) was used for $9MOG^{\bullet+}$ and CASSCF(12,8)/6-31+G(d,p) for $^1O_2$.
[c] CASPT2(9,7)/6-31G(d,p) was used for $9MOG^{\bullet+}$ and CASPT2(12,8)/6-31G(d,p) for $^1O_2$.
[d, e] before and after the annihilation of spin contamination.
[f] calculated at DLPNO-CCSD(T)/aug-cc-pVTZ.

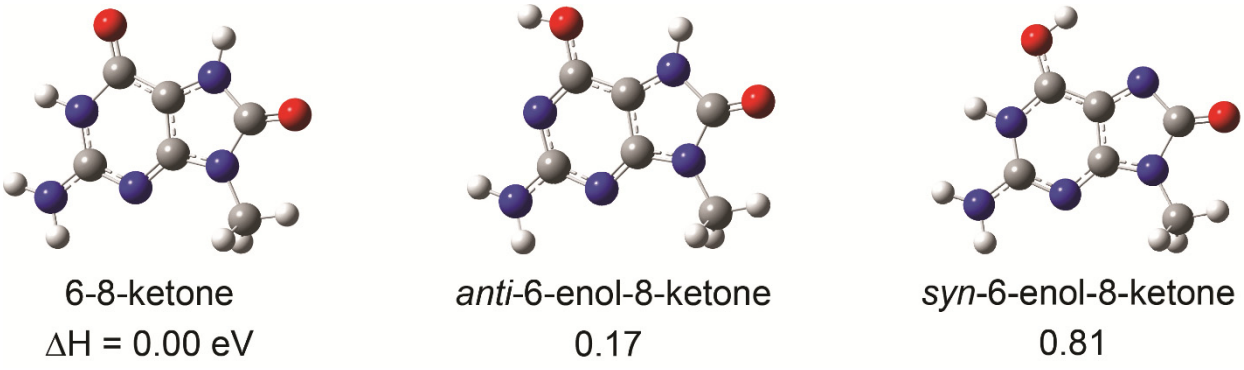

Figure S1. The keto-enol tautomers of 9MOG$^{\bullet+}$. Relative enthalpies (ΔH with respect to the global energy minimum, eV) were calculated at the ωB97XD/6-31+G(d,p) level of theory, including thermal corrections at 298 K.

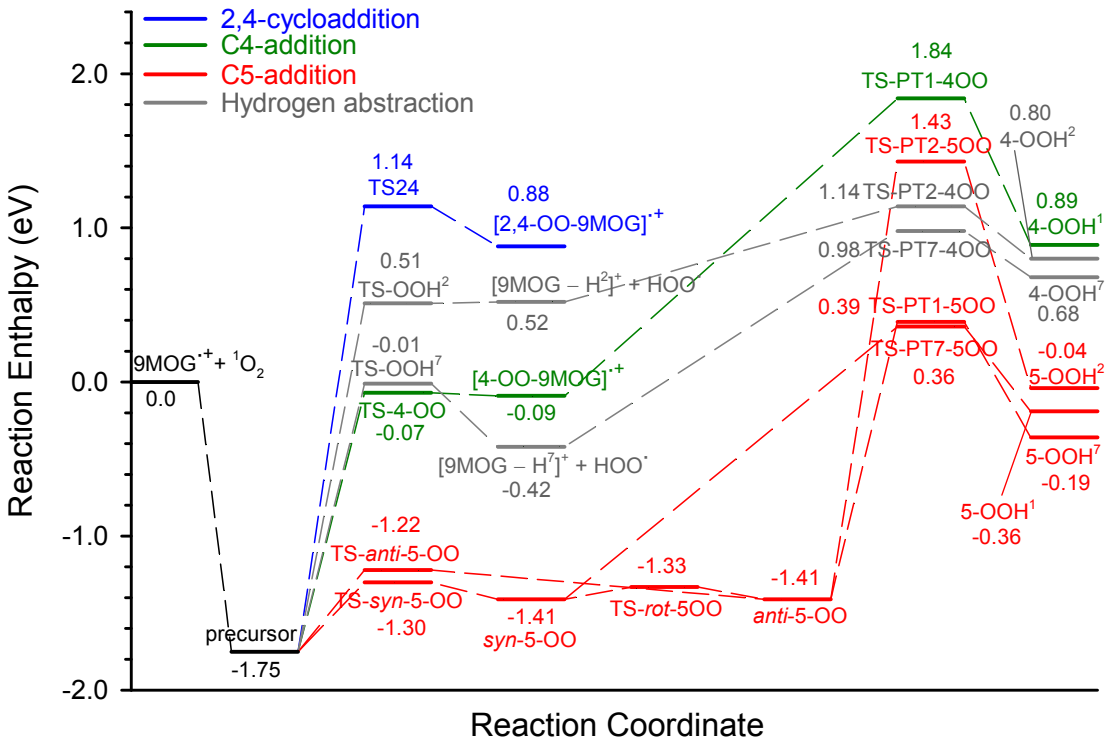

Figure S2. Schematic PES for 9MOG$^{\bullet+}$ + $^1O_2$ calculated at the ωB97XD/6-31+G(d,p) level of theory. Reaction enthalpies were calculated at 298 K including thermal corrections.

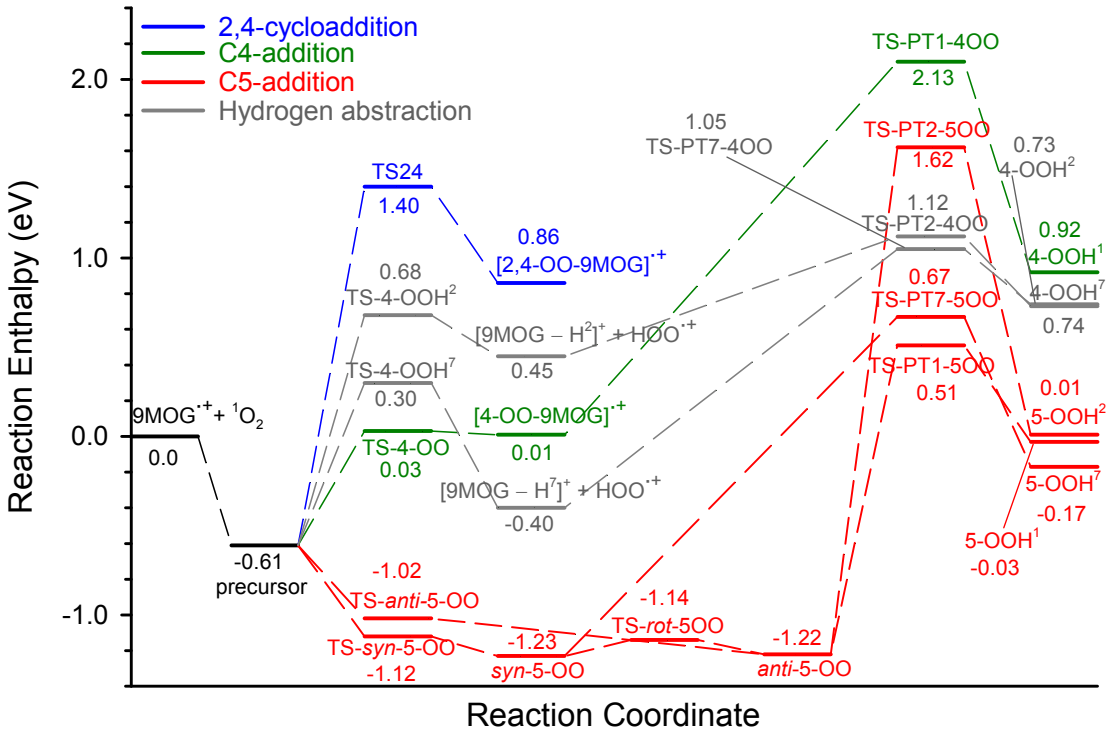

Figure S3. Schematic PES for 9MOG$^{\bullet+}$ + $^1O_2$ calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ level of theory. Reaction enthalpies were calculated at 298 K including thermal corrections.

Cartesian coordinates for the structures in Scheme 2, optimized at ωB97XD/ 6-31+G(d,p).

9MOG$^{\bullet+}$

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

OG$^{\bullet+}$

O1 1.999968 -1.393160 1.505235
C2 2.571296 -0.216394 2.058360
H3 1.924619 0.191971 2.844869
H4 3.560533 -0.415057 2.489753
C5 2.720916 0.822154 0.961937
H6 3.120797 1.741767 1.396892
O7 1.442824 1.148352 0.397194
C8 1.260319 0.516949 -0.831928
H9 0.955762 1.269079 -1.563574
N10 0.065548 -0.379867 -0.710495
C11 -0.019693 -1.792260 -0.678809
N12 -1.357665 -2.073564 -0.289576
C13 -2.037423 -0.935473 -0.126702
C14 -3.409217 -0.679136 0.237547
O15 -4.263303 -1.498101 0.490782
N16 -3.658796 0.711321 0.271446
H17 -4.607417 0.960512 0.529607
C18 -2.734620 1.677753 -0.013317
N19 -3.103381 2.953070 0.044959
H20 -4.034883 3.254481 0.285826
H21 -2.400964 3.652493 -0.151658
N22 -1.465133 1.418501 -0.352311
C23 -1.142432 0.142945 -0.394467
C24 3.581270 0.411225 -0.235589
H25 4.346896 -0.318628 0.050165
C26 2.563005 -0.199091 -1.206993
H27 2.492022 -1.271651 -1.046283
H28 2.829453 -0.012872 -2.248783
O29 4.166552 1.597817 -0.734594
H30 2.152624 -2.136608 2.093578
H31 4.810351 1.382742 -1.415747
H32 -1.714739 -3.018184 -0.208723
O33 0.789008 -2.627197 -0.961657

Zero-point correction= 0.260489 (Hartree/Particle)
Thermal correction to Energy= 0.278033
Thermal correction to Enthalpy= 0.278977
Thermal correction to Gibbs Free Energy= 0.214599
Sum of electronic and zero-point Energies= -1038.032249
Sum of electronic and thermal Energies= -1038.014704
Sum of electronic and thermal Enthalpies= -1038.013760
Sum of electronic and thermal Free Energies= -1038.078139

Cartesian coordinates for the structures in Scheme 3, optimized at ωB97XD/ 6-31+G(d,p).

9MOG$^{\bullet+}$

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

$^1O_2$

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

precursor complex

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

TS-24

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]$^{\bullet+}$

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

TS-4OO

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

[4-OO-9MOG]$^{\bullet+}$

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

TS-PT1-4OO

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^{1}-9MOG]$^{\bullet+}$
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

TS-*syn*-5OO
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]$^{\bullet+}$**
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

TS-PT7-5OO

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^{7}-9MOG]$^{\bullet+}$

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

TS-*rot*-5OO

C1 -0.244999 0.646026 -0.056414
C2 -0.087072 -0.848385 0.130393
C3 1.159979 -1.347486 -0.584476
C4 1.971125 0.942440 -0.265822
C5 -2.285113 -0.328165 -0.271219
H6 3.094985 -0.707498 -0.849994
H7 -1.606080 -2.314521 -0.218501
O8 1.305280 -2.439324 -1.048191
O9 -3.466205 -0.392261 -0.406577
N10 -1.340704 -1.339135 -0.252186
N11 -1.534366 0.907391 -0.154681
N12 0.747218 1.487281 -0.140227
N13 2.182829 -0.382918 -0.545109
N14 3.011464 1.748646 -0.183082
H15 3.967988 1.431504 -0.248590
H16 2.837750 2.730824 -0.012557
O17 0.185662 -1.187338 1.558960
O18 0.349690 -0.153608 2.335136
C19 -2.152369 2.218836 -0.317998
H20 -1.932627 2.612480 -1.312146
H21 -1.764720 2.892121 0.446423
H22 -3.227101 2.086883 -0.199061

Zero-point correction= 0.158726 (Hartree/Particle)
Thermal correction to Energy= 0.171204
Thermal correction to Enthalpy= 0.172148
Thermal correction to Gibbs Free Energy= 0.119533
Sum of electronic and zero-point Energies= -806.790008
Sum of electronic and thermal Energies= -806.777530
Sum of electronic and thermal Enthalpies= -806.776586
Sum of electronic and thermal Free Energies= -806.829201

TS-*anti*-5OO

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]$^{\bullet+}$**
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

TS-PT1-5OO
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^{1}-9MOG]$^{\bullet+}$
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

TS-PT2-5OO

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-OOH^2-9MOG]$^{\bullet+}$

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

TS-OOH^2

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^2]$^+$ + HOO$^\bullet$

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

TS-PT2-4OO
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^{2}-9MOG]$^{\bullet+}$
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

TS-OOH^{7}
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^{7}]$^{+}$ + HOO$^{\bullet}$

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

TS-PT7-4OO

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^{7}-9MOG]$^{\bullet+}$

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

Cartesian coordinates for the 9MOG^{+} conformers in Figure S1, optimized at ωB97XD/6-31+G(d,p).

6,8-ketone

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

***anti*-6-enol-8-ketone**

C1 0.232086 -0.557481 -0.000137
C2 0.009267 0.860789 0.000218
C3 -1.348444 1.289850 0.000927
C4 -1.967282 -0.923048 -0.000523
C5 2.235724 0.482980 -0.001379
H6 1.399777 2.458880 -0.000071
O7 -1.585719 2.583347 0.002165
O8 3.412598 0.694399 -0.002770
N9 1.204251 1.464873 0.000128
N10 1.570968 -0.754669 -0.003205
N11 -0.715750 -1.455620 0.000550
N12 -2.304951 0.402351 0.000340
N13 -2.978005 -1.777275 -0.002250
H14 -3.928768 -1.435897 -0.003100
H15 -2.795273 -2.771061 -0.002700
C16 2.258673 -2.041940 0.004958
H17 2.091153 -2.544037 0.958784
H18 1.881801 -2.657408 -0.812299
H19 3.321839 -1.848328 -0.131788
H20 -2.541307 2.751353 0.002686

Zero-point correction= 0.152061 (Hartree/Particle)
Thermal correction to Energy= 0.162891
Thermal correction to Enthalpy= 0.163835
Thermal correction to Gibbs Free Energy= 0.114954
Sum of electronic and zero-point Energies= -656.524911
Sum of electronic and thermal Energies= -656.514081
Sum of electronic and thermal Enthalpies= -656.513137
Sum of electronic and thermal Free Energies= -656.562018

***syn*-6-enol-8-ketone**

C1 0.267212 -0.558194 0.000701
C2 0.095800 0.877334 0.000540
C3 -1.210859 1.350003 -0.001166
C4 -1.939427 -0.946965 0.000939
C5 2.227403 0.536462 0.001882
O6 -1.606313 2.593075 -0.003525
O7 3.418072 0.677928 0.004350
N8 1.242845 1.543595 0.000201
N9 1.577268 -0.761992 0.003143
N10 -0.712045 -1.452628 0.000079
N11 -2.202778 0.413279 -0.000537
N12 -2.981095 -1.774663 0.002837
H13 -3.942841 -1.472377 0.004035
H14 -2.788847 -2.766834 0.003368
C15 2.287922 -2.033328 -0.006905
H16 1.916698 -2.666812 0.799448
H17 2.146645 -2.530770 -0.967773
H18 3.344847 -1.816203 0.144219
H19 -0.850423 3.203708 -0.004026
H20 -3.157826 0.756251 -0.001880

Zero-point correction= 0.150990 (Hartree/Particle)
Thermal correction to Energy= 0.162005
Thermal correction to Enthalpy= 0.162950
Thermal correction to Gibbs Free Energy= 0.113866
Sum of electronic and zero-point Energies= -656.501735
Sum of electronic and thermal Energies= -656.490720
Sum of electronic and thermal Enthalpies= -656.489776
Sum of electronic and thermal Free Energies= -656.538859