Supporting Information

pH-Dependent Singlet O_2 Oxidation Kinetics of Guanine and 9-Methylguanine: An On-line Mass Spectrometry and Spectroscopy Study Combined with Theoretical Exploration

Wenchao Lu,[ab] Yan Sun,[ab] Wenjing Zhou,[a] and Jianbo Liu*[ab]

[a] Department of Chemistry and Biochemistry, Queens College of the City University of New York, 65-30 Kissena Blvd., Queens, NY 11367, USA; [b] Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, 365 5th Ave., New York, NY 10016, USA

*E-mail: jianbo.liu@qc.cuny.edu

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Calibration of [$^1O_2$] in solution In the experiment, chemically generated $^1O_2$ was continuously bubbled into the reaction vessel. $^1O_2$ had a longer lifetime in the interior of bubbles (because of reduced encounters with water) than in bulk solution. After diffusing into the bulk water, $^1O_2$ could travel ~ 150 nm within a lifetime of ~ 2 μs.[1] Therefore, $^1O_2$ reactions occurred both at the gas/solution interface and in the bulk solution. Considering the steady concentration of airborne $^1O_2$ (determined on the basis of its emission intensity) and the continuously bubbling of $^1O_2$ into the solution, a quasi-steady-state [$^1O_2$] may be assumed for the solution reaction. To validate this assumption and determine the average [$^1O_2$] in solution, 3-(10-(2-carboxy-ethyl)-anthracen-9-yl)-propionic acid (ADPA, Aldrich) was used as a calibration compound.

The detailed calibration procedure has been reported in our previous work.[2] ADPA is known to react with $^1O_2$ chemically (*i.e.* without physical quenching), producing endoperoxide *via* a [4 + 2] cycloaddition accompanied by bleaching of the absorption band of ADPA.[3] Fig. S1a shows the absorption changes of ADPA throughout the reaction. pH of the ADPA solution (0.1 mM) was maintained at 10.0 using borax/NaOH buffer. Shown in the inset of Fig. S1a is the plot of $ln\ (A_t/A_0)$ *vs.* reaction time, where A_t and A_0 are the ADPA peak absorption (at 378 nm) at different reaction times and time zero, respectively. The observation of a linear relationship between $ln\ (A_t/A_0)$ and reaction time indicates that the consumption of ADPA followed first-order rate law. Accordingly, an average [$^1O_2$] in solution could be extracted using the reaction rate k_r ($8.2 \times 10^7\ M^{-1}\cdot s^{-1}$) for ADPA + $^1O_2$.[3]

During the experiment, emission of airborne $^1O_2$ was continuously monitored. Fig. S1b presents the correlation between the output of the emission detector and the corresponding ADPA-calibrated [$^1O_2$] in solution. It shows that [$^1O_2$] in solution increases linearly with the growth of airborne $^1O_2$ emission. The calibration curve crosses the x-axis at ~ 50 mV. This indicates a threshold airborne concentration below which all of the $^1O_2$ quenched in bubbles and/or during diffusion before reaching aqueous substrates. The calibration curve of Fig. S1b was used to determine [$^1O_2$] in the solution-phase reactions for guanine and 9MG.

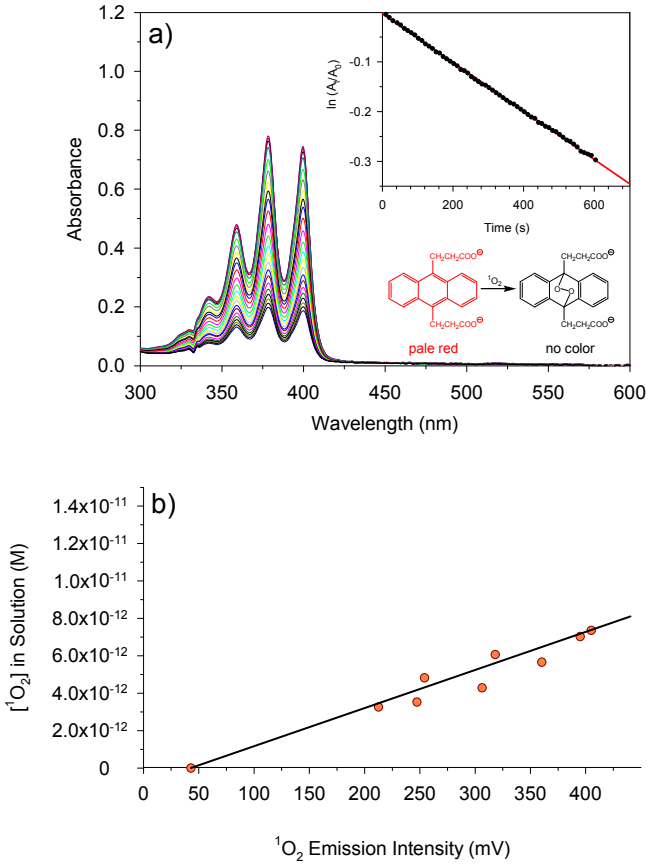


Fig. S1 (a) UV-Vis absorption spectra of ADPA over the course of the reaction with $^1O_2$. Inset shows the linearity of *ln* (A_t/A_0) against reaction time; and (b) the linear relationship between the emission intensity of airborne $^1O_2$ and the concentration of $^1O_2$ in solution determined using ADPA trapping.

1. E. Skovsen, J. W. Snyder, J. D. C. Lambert and P. R. Ogilby, *J. Phys. Chem. B*, 2005, **109**, 8570-8573.
2. F. Liu, W. Lu, X. Yin and J. Liu, *J. Am. Soc. Mass. Spectrom.*, 2016, **27**, 59-72.
3. B. A. Lindig, M. A. J. Rodgers and A. P. Schaap, *J. Am. Chem. Soc.*, 1980, **102**, 5590-5593.

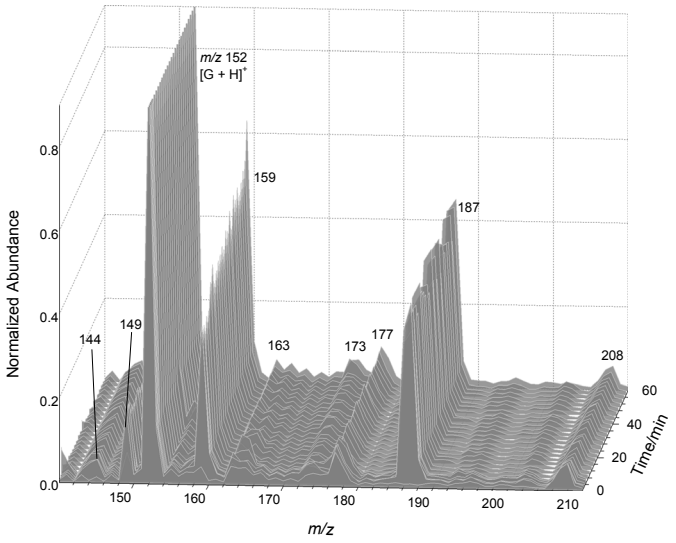


Fig. S2 MS spectra recorded for guanine + $^1O_2$ at pH 3.0.

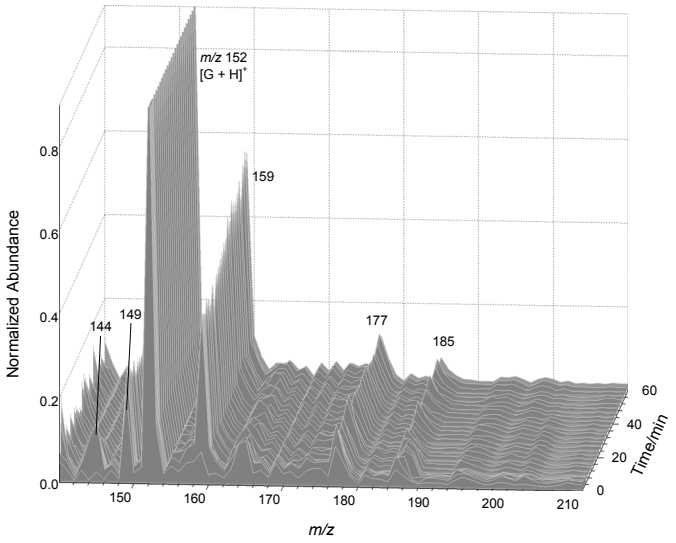


Fig. S3 MS spectra recorded for guanine + $^1O_2$ at pH 7.0.

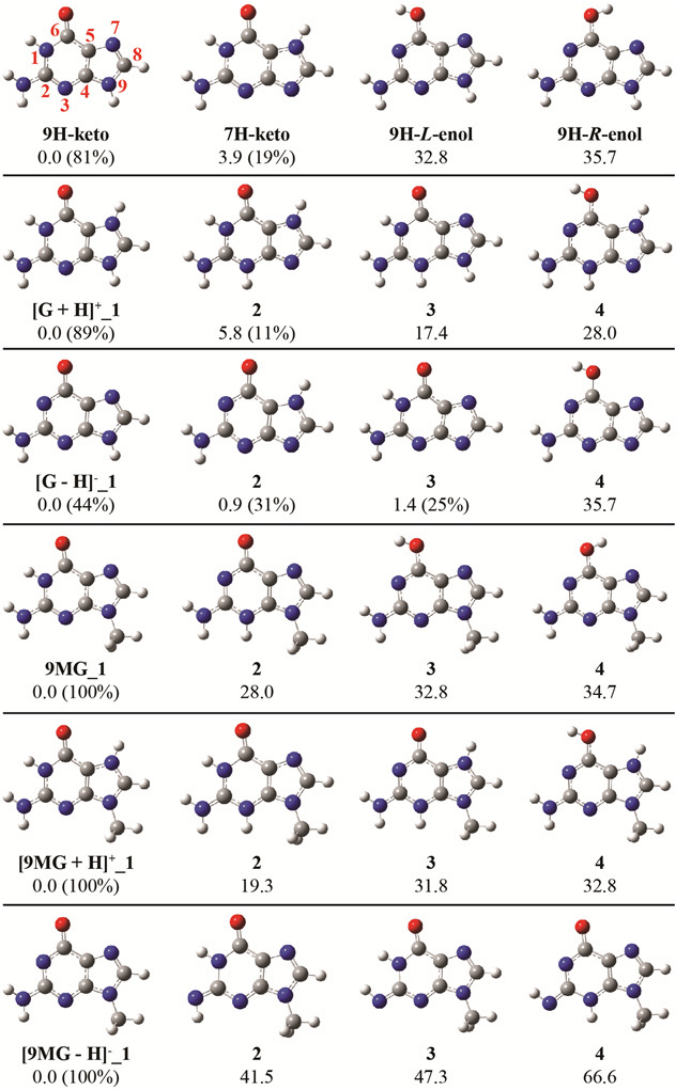


Fig. S4 Stable conformers of neutral, protonated and deprotonated guanine and 9MG. Relative energies (kJ/mol, including thermal corrections at 298 K) were evaluated at SMD-ωB97XD/6-31+G(d,p). Populations are indicated in parentheses.

Cartesian coordinates for the structures of neutral, protonated and deprotonated guanine and 9MG in Fig. S4, optimized at SMD-ωB97XD/6-31+G(d,p).

9HG_keto
C1 -0.234529 1.431728 0.000050
C2 0.836586 0.497799 -0.000488
C3 -1.671326 -0.572112 -0.002017
C4 2.704941 -0.512212 0.001429
N5 -1.474573 0.787038 -0.003096
N6 2.206804 0.698503 0.000939
N7 1.742151 -1.488652 0.000859
N8 -0.682851 -1.444768 0.001910
C9 0.534298 -0.856696 -0.000389
N10 -2.951425 -0.997522 -0.045544
H11 -3.114562 -1.977565 0.135158
H12 -3.702434 -0.357532 0.170540
O13 -0.182028 2.671557 0.002902
H14 3.756098 -0.759523 0.002125
H15 1.903313 -2.487643 0.000445
H16 -2.286750 1.396582 -0.008467

7HG_keto
C1 -0.201251 1.417254 -0.000309
C2 0.817960 0.434973 -0.001190
H3 -2.250909 1.451000 -0.012963
C4 -1.691203 -0.539563 -0.002538
C5 2.645525 -0.749604 0.002586
N6 -1.457481 0.817171 -0.005034
N7 2.193108 0.518093 0.001877
N8 1.677113 -1.656828 0.000943
N9 -0.736136 -1.441113 0.001813
C10 0.521446 -0.920605 -0.001328
N11 -2.991755 -0.918620 -0.053968
H12 -3.177607 -1.890376 0.150541
H13 -3.704831 -0.259703 0.226942
O14 -0.084518 2.653639 0.003235
H15 3.702352 -0.972572 0.004149
H16 2.758329 1.356893 0.002714

9H_*L*_enol
C1 -0.318618 1.304090 0.000320
C2 0.805646 0.475752 -0.002532
C3 -1.671215 -0.560640 -0.003391
C4 2.689524 -0.499850 0.000213
N5 -1.538337 0.789974 0.000256
N6 2.174946 0.703683 -0.003248
N7 1.749985 -1.498717 0.003918
N8 -0.681838 -1.462039 0.003019
C9 0.526365 -0.890286 0.001424
N10 -2.948030 -1.031393 -0.059454
H11 -3.092094 -2.000732 0.183091
H12 -3.688996 -0.390126 0.182103
O13 -0.168502 2.633860 0.004705
H14 3.745601 -0.726938 -0.000142
H15 -1.041628 3.054724 0.003806
H16 1.937843 -2.492766 0.005859

9H_*R*_enol
C1 -0.291599 1.315429 0.000117
C2 0.805257 0.449309 -0.003300
C3 -1.699014 -0.505712 -0.003367
C4 2.659738 -0.582360 0.000519
N5 -1.525354 0.838743 0.000265
N6 2.181353 0.636067 -0.003625
N7 1.689882 -1.552004 0.004263
N8 -0.739672 -1.440766 0.002919
C9 0.484773 -0.907646 0.001065
N10 -2.989813 -0.937853 -0.059130
H11 -3.161821 -1.903667 0.179225
H12 -3.711107 -0.275917 0.185911
O13 -0.186655 2.653349 0.004864
H14 3.708456 -0.841110 0.000833
H15 0.742652 2.922069 0.005160
H16 1.845353 -2.551602 0.006909

$[G + H]^+$_1
C1 -0.269053 1.439589 -0.000001
C2 0.781354 0.477710 -0.000002
H3 -2.316681 1.414950 -0.000019
C4 -1.712516 -0.560249 -0.000001
H5 1.843422 -2.526319 0.000002
C6 2.685727 -0.613141 0.000008
N7 -1.506779 0.800552 0.000002
N8 2.158581 0.597787 0.000006
N9 1.700568 -1.521689 -0.000001
N10 -0.723180 -1.443835 -0.000005
C11 0.487080 -0.868869 -0.000007
N12 -2.980863 -0.977439 -0.000055
H13 -3.169310 -1.968938 0.000130
H14 -3.753199 -0.327607 0.000282
O15 -0.176344 2.668380 -0.000004
H16 3.740607 -0.838340 0.000015
H17 2.692075 1.461335 0.000010

$[G + H]^+$_2
C1 -0.169173 1.445261 -0.000009
C2 0.847930 0.448883 -0.000009
H3 -2.231542 1.514473 -0.000073
C4 -1.741970 -0.463154 -0.000006
C5 2.664637 -0.754393 0.000033

N6 -1.451984 0.860729 -0.000011
N7 2.221574 0.512955 0.000033
N8 1.681250 -1.655154 -0.000011
N9 -0.735090 -1.350370 -0.000046
C10 0.564964 -0.897100 -0.000034
N11 -2.998793 -0.865288 -0.000045
H12 -3.225052 -1.851461 0.000210
H13 -3.753198 -0.191769 0.000537
O14 -0.047342 2.665081 -0.000011
H15 3.717404 -0.992588 0.000067
H16 2.793128 1.349121 0.000061
H17 -0.939032 -2.345517 0.000006

$[G + H]^+$_3
C1 0.203026 1.458603 -0.000002
C2 -0.864679 0.506916 -0.000003
H3 2.269951 1.463597 0.000004
C4 1.727036 -0.494734 0.000005
H5 -1.904707 -2.492527 -0.000001
C6 -2.727824 -0.514839 -0.000005
N7 1.471598 0.832844 0.000002
N8 -2.231934 0.695666 -0.000006
N9 -1.757378 -1.489679 -0.000002
N10 0.690682 -1.353114 0.000003
C11 -0.577269 -0.837163 0.000000
N12 2.967685 -0.940465 0.000009
H13 3.159462 -1.934308 0.000010
H14 3.745398 -0.293555 0.000008
O15 0.137459 2.681787 -0.000004
H16 -3.776031 -0.771713 -0.000007
H17 0.859935 -2.355262 0.000004

$[G + H]^+$_4
C1 -0.259122 1.322556 0.000000
C2 0.816340 0.425083 0.000007
C3 -1.739635 -0.447003 -0.000011
C4 2.647457 -0.753944 -0.000015
N5 -1.505793 0.875462 -0.000019
N6 2.191241 0.509735 -0.000008
N7 1.681018 -1.672054 0.000006
N8 -0.739910 -1.366662 0.000021
C9 0.551787 -0.931126 0.000019
N10 -2.997319 -0.878333 -0.000221
H11 -3.219846 -1.863926 0.001030
H12 -3.747093 -0.202628 0.000306
O13 -0.023287 2.621178 0.000035
H14 3.703938 -0.976648 -0.000041
H15 2.755162 1.350797 -0.000018
H16 -0.860121 3.113190 0.000048
H17 -0.951356 -2.360640 -0.000051

$[G - H]^-$_1
C1 -0.291592 1.415891 -0.000004
C2 0.799185 0.491337 -0.003321
C3 -1.685511 -0.477162 -0.006920
H4 1.866118 -2.501760 0.006947
C5 2.671429 -0.529776 0.002565
N6 -1.539650 0.861045 -0.001941
N7 2.176183 0.683500 -0.001508
N8 1.706733 -1.503539 0.004214
N9 -0.728647 -1.416659 -0.000773
C10 0.496207 -0.860301 -0.000278
N11 -2.983849 -0.938644 -0.071446
H12 -3.118514 -1.889898 0.241892
H13 -3.688763 -0.288480 0.245693
O14 -0.141866 2.677490 0.006144
H15 3.722394 -0.779637 0.004241

$[G - H]^-$_2
C1 -0.257224 1.402862 -0.001236
C2 0.780241 0.427938 -0.004245
C3 -1.703463 -0.444372 -0.008367
C4 2.610248 -0.767902 0.005581
N5 -1.518454 0.893931 -0.005035
N6 2.160321 0.503625 0.001584
N7 1.640566 -1.671550 0.003525
N8 -0.782647 -1.410981 -0.003731
C9 0.481406 -0.923425 -0.002553
N10 -3.023244 -0.855149 -0.070557
H11 -3.186177 -1.799851 0.249925
H12 -3.692909 -0.182558 0.275980
O13 -0.040066 2.655964 0.005979
H14 3.666882 -0.993443 0.009696
H15 2.729693 1.338405 0.000989

$[G - H]^-$_3
C1 -0.163242 1.409575 -0.000323
C2 0.876562 0.453650 -0.000540
H3 -2.218521 1.434941 -0.020063
C4 -1.650662 -0.550481 -0.003549
C5 2.666875 -0.651296 0.003040
N6 -1.423055 0.805379 -0.007573
N7 2.247137 0.612836 0.002708
N8 1.718992 -1.627247 0.001215
N9 -0.697414 -1.444349 0.002783
C10 0.569181 -0.914471 -0.001299
N11 -2.964432 -0.932776 -0.068326
H12 -3.127018 -1.899657 0.178756
H13 -3.650300 -0.289669 0.305099
O14 -0.085896 2.659233 0.003997
H15 3.722113 -0.898248 0.004613

[G – H]⁻_4
C1 -0.246303 1.285609 -0.000981
C2 0.849421 0.431366 -0.002536
C3 -1.651946 -0.532487 -0.007182
C4 2.650776 -0.649472 0.003901
N5 -1.487719 0.814467 -0.004170
N6 2.219332 0.612515 0.000746
N7 1.723588 -1.642370 0.003634
N8 -0.698356 -1.456826 -0.001403
C9 0.557962 -0.946352 -0.000893
N10 -2.962145 -0.966661 -0.073140
H11 -3.105580 -1.916506 0.241739
H12 -3.646981 -0.311111 0.276889
O13 -0.067956 2.624295 0.004992
H14 3.710215 -0.879587 0.006372
H15 -0.936366 3.052984 0.001534

9MG_1
C1 -1.130432 1.366537 0.000875
C2 0.241414 0.997063 -0.001077
H3 -2.959548 0.438671 -0.004438
C4 -1.546751 -1.064071 -0.001877
C5 2.359148 0.896134 0.000086
N6 -1.963105 0.243970 0.000419
N7 1.385500 1.773749 -0.000548
N8 1.925935 -0.405795 0.000059
N9 -0.276917 -1.415763 0.000943
C10 0.562575 -0.354584 -0.000815
N11 -2.515236 -2.005900 -0.054389
H12 -2.233634 -2.954567 0.148069
H13 -3.461809 -1.753510 0.194714
O14 -1.629272 2.503642 0.003123
H15 3.414849 1.128636 0.000417
C16 2.757222 -1.598271 0.002873
H17 2.562901 -2.191816 0.897670
H18 2.558060 -2.199230 -0.885866
H19 3.801056 -1.286002 -0.001323

9MG_2
C1 -1.166849 1.361923 -0.000090
C2 0.228567 1.002351 -0.002188
C3 -1.670299 -0.943086 -0.001851
C4 2.355998 0.894201 0.002585
N5 -2.066278 0.317470 0.001547
N6 1.380338 1.769836 0.001567
N7 1.919209 -0.410261 -0.000344
N8 -0.358138 -1.329064 -0.003937
C9 0.567191 -0.328571 -0.003472
N10 -2.585498 -1.930940 -0.039254
H11 -2.309879 -2.884773 0.148276
H12 -3.547918 -1.678206 0.128556
O13 -1.576364 2.543730 0.002229
H14 3.412844 1.119817 0.005140
C15 2.733556 -1.616990 0.002187
H16 2.524565 -2.207781 0.895842
H17 2.527148 -2.209676 -0.890785
H18 3.781131 -1.318970 0.003362
H19 -0.093394 -2.308511 -0.008300

9MG_3
C1 -1.196022 1.172398 0.001688
C2 0.185254 0.969742 -0.005257
H3 -2.659508 2.371906 0.017376
C4 -1.515894 -1.109405 -0.005981
C5 2.303367 0.982042 -0.005084
N6 -2.032434 0.145413 -0.000173
N7 1.287737 1.810258 -0.005013
N8 1.946975 -0.343478 -0.006596
N9 -0.219878 -1.440267 -0.002977
C10 0.580068 -0.368450 -0.005286
N11 -2.425037 -2.124166 -0.062532
H12 -2.096247 -3.044310 0.192527
H13 -3.373871 -1.901419 0.200327
O14 -1.691333 2.416504 0.012818
H15 3.344975 1.272427 -0.005032
C16 2.842065 -1.488252 0.015736
H17 2.719030 -2.046745 0.945445
H18 2.635043 -2.142542 -0.832717
H19 3.866664 -1.124125 -0.054332

9MG_4
C1 -1.188292 1.187072 0.002055
C2 0.189199 0.955971 -0.005784
H3 -1.043371 3.090754 0.016220
C4 -1.546649 -1.086133 -0.006023
C5 2.306742 0.937777 -0.005928
N6 -2.042424 0.175946 0.000550
N7 1.303410 1.780969 -0.005587
N8 1.930183 -0.382142 -0.007430
N9 -0.256173 -1.443678 -0.003466
C10 0.562808 -0.387554 -0.005957
N11 -2.472874 -2.086026 -0.063339
H12 -2.159223 -3.010676 0.194547
H13 -3.416676 -1.847228 0.203603
O14 -1.734724 2.413265 0.013741
H15 3.352557 1.212661 -0.006041
C16 2.809309 -1.539154 0.016986
H17 2.672499 -2.098367 0.944274
H18 2.599307 -2.187943 -0.834929
H19 3.839151 -1.188668 -0.044791

[9MG + H]$^+$_1
C1 -1.147757 1.370533 0.000012
C2 0.215418 0.959020 0.000030
H3 -2.982918 0.465028 -0.000028
C4 -1.586253 -1.056162 0.000023
C5 2.400356 0.787498 -0.000030
N6 -1.987663 0.259525 0.000016
N7 1.404250 1.659375 -0.000021
N8 1.911743 -0.460464 0.000021
N9 -0.312476 -1.424091 0.000078
C10 0.532195 -0.382599 0.000054
N11 -2.550930 -1.979834 -0.000181
H12 -2.293101 -2.955371 0.000315
H13 -3.528070 -1.726427 0.000238
O14 -1.599187 2.517874 -0.000008
H15 3.449980 1.038814 -0.000071
C16 2.700548 -1.688663 -0.000025
H17 2.468139 -2.267798 0.893554
H18 2.468055 -2.267781 -0.893593
H19 3.754597 -1.416307 -0.000072
H20 1.515304 2.667502 -0.000051

[9MG + H]$^+$_2
C1 1.104428 1.408304 0.000023
C2 -0.270149 1.016534 -0.000007
H3 2.967244 0.516949 0.000039
C4 1.631212 -1.013944 0.000020
C5 -2.387923 0.892663 -0.000064
N6 1.975148 0.293090 0.000059
N7 -1.420606 1.775654 -0.000068
N8 -1.941065 -0.409317 -0.000001
N9 0.324899 -1.337633 0.000106
C10 -0.594641 -0.320851 0.000031
N11 2.557777 -1.953224 -0.000057
H12 2.296894 -2.931149 -0.000419
H13 3.539081 -1.706681 -0.000281
O14 1.580722 2.537726 0.000017
H15 -3.446226 1.109952 -0.000110
C16 -2.754682 -1.619522 0.000023
H17 -2.544408 -2.207918 -0.894305
H18 -2.544707 -2.207676 0.894582
H19 -3.801144 -1.319188 -0.000185
H20 0.044946 -2.315194 0.000121

[9MG + H]$^+$_3
C1 -1.183293 1.366397 0.000006
C2 0.204236 0.957795 0.000017
C3 -1.711828 -0.930457 -0.000001
C4 2.396229 0.782309 -0.000024
N5 -2.088785 0.340410 -0.000015
N6 1.396635 1.650813 -0.000018
N7 1.904064 -0.468190 0.000012
N8 -0.400371 -1.341503 0.000052
C9 0.539328 -0.362763 0.000036
N10 -2.635870 -1.893902 -0.000011
H11 -2.384979 -2.872067 -0.000096
H12 -3.610224 -1.632130 -0.000157
O13 -1.531848 2.559149 0.000010
H14 3.447058 1.027715 -0.000050
C15 2.685927 -1.704669 -0.000017
H16 2.448208 -2.279204 0.895494
H17 2.448189 -2.279174 -0.895542
H18 3.740766 -1.437019 -0.000023
H19 -0.152051 -2.326173 0.000093
H20 1.504506 2.659799 -0.000038

[9MG + H]$^+$_4
C1 1.220801 1.174864 -0.000029
C2 -0.158545 0.935596 0.000234
C3 1.551174 -1.109410 0.000217
C4 -2.350667 0.878748 -0.000022
N5 2.055222 0.156258 -0.000005
N6 -1.311399 1.700130 0.000138
N7 -1.935407 -0.393933 -0.000090
N8 0.251076 -1.450635 -0.000088
C9 -0.550524 -0.392687 0.000074
N10 2.455857 -2.102888 0.004558
H11 2.149933 -3.063229 -0.014224
H12 3.440156 -1.888532 -0.014091
O13 1.673784 2.424755 -0.000431
H14 -3.385031 1.187691 -0.000058
C15 -2.789617 -1.577296 -0.000249
H16 -2.588419 -2.168232 -0.893677
H17 -2.588433 -2.168443 0.893045
H18 -3.827271 -1.249069 -0.000210
H19 2.644016 2.418724 -0.000512
H20 -1.378405 2.711624 0.000233

[9MG – H]$^-$_1
C1 -1.190857 1.319433 0.000905
C2 0.199251 0.983609 -0.002827
C3 -1.587902 -0.999143 -0.007401
C4 2.327108 0.897920 0.000700
N5 -2.055509 0.262396 -0.002194
N6 1.345055 1.768339 -0.001351
N7 1.904677 -0.406387 0.001114
N8 -0.311909 -1.409633 -0.001908
C9 0.533861 -0.362272 -0.001549
N10 -2.545918 -1.990753 -0.073125
H11 -2.246048 -2.900256 0.249531
H12 -3.464072 -1.718220 0.248224
O13 -1.630190 2.512073 0.007941

H14 3.381136 1.139734 0.001331
C15 2.740766 -1.592440 0.004293
H16 2.550236 -2.191640 0.897058
H17 2.547525 -2.197925 -0.883623
H18 3.784597 -1.278652 0.001477

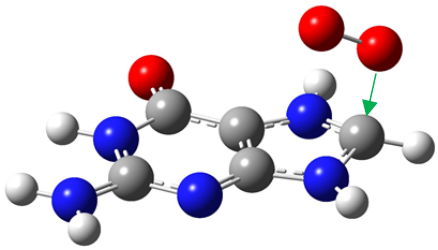
[9MG – H]⁻_2
C1 -1.236797 -1.271822 -0.002878
C2 0.150437 -0.982692 0.003078
H3 -3.009908 -0.254494 -0.006428
C4 -1.559756 1.209951 0.001347
C5 2.274819 -1.000754 0.006594
N6 -2.005585 -0.122950 -0.003929
N7 1.256708 -1.822141 0.004648
N8 1.910886 0.326173 0.008254
N9 -0.221859 1.460342 0.002486
C10 0.539138 0.357838 0.004214
N11 -2.497686 2.120922 0.004411
H12 -2.041670 3.030867 0.008411
O13 -1.788082 -2.398272 -0.007553
H14 3.316907 -1.289360 0.007651
C15 2.803726 1.469964 -0.013618
H16 2.677186 2.036856 -0.938506
H17 2.605294 2.122843 0.838726
H18 3.830193 1.108136 0.047066

[9MG – H]⁻_3
C1 -1.221084 1.269201 -0.002607
C2 0.163085 0.977189 0.002857
H3 -2.995777 0.274960 -0.005606
C4 -1.553412 -1.221173 0.001451
C5 2.287048 0.986592 0.005938
N6 -1.994442 0.119104 -0.002949
N7 1.272930 1.812580 0.003965
N8 1.918110 -0.338840 0.007950
N9 -0.215432 -1.465578 0.002499
C10 0.545540 -0.365949 0.004144
N11 -2.419585 -2.201744 0.004062
H12 -3.367308 -1.830434 0.002724
O13 -1.773756 2.394861 -0.007355
H14 3.330345 1.270947 0.006689
C15 2.807264 -1.485316 -0.012576
H16 2.609495 -2.134916 0.842435
H17 2.676553 -2.054944 -0.935180
H18 3.835023 -1.126419 0.043859

[9MG – H]⁻_4
C1 -1.275161 1.253036 -0.003909
C2 0.146083 0.978689 0.003259
C3 -1.679589 -1.106932 0.001645
C4 2.280335 0.993715 0.008988
N5 -2.113626 0.189538 -0.004159
N6 1.255312 1.810886 0.005910
N7 1.913245 -0.334634 0.010708
N8 -0.307718 -1.378306 0.002404
C9 0.555035 -0.331429 0.005274
N10 -2.465995 -2.149080 0.005494
H11 -3.425753 -1.811692 0.003799
O12 -1.726872 2.437415 -0.010536
H13 3.322972 1.277998 0.010796
C14 2.789230 -1.495267 -0.017557
H15 2.575793 -2.147478 0.831708
H16 2.653062 -2.049586 -0.948340
H17 3.819941 -1.148504 0.048554
H18 0.004827 -2.339762 0.009077

Cartesian coordinates for the structures in Fig. 3, optimized at SMD-ωB97XD/aug-cc-pVQZ//SMD-ωB97XD/6-31+G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

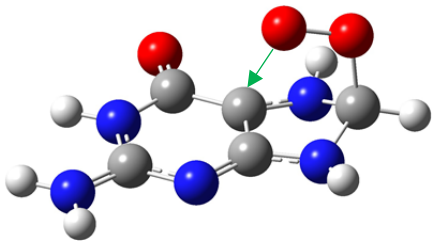
Guanine
TS1$^+$ (open-shell)



C1 0.207163 0.671294 -0.379216
C2 0.072796 -0.730679 -0.501719
C3 -2.084904 -0.698356 0.055904
C4 -0.925708 1.467555 -0.005115
C5 2.203017 -0.166434 -0.828780
N6 -2.044319 0.664580 0.202227
N7 -1.024094 -1.436401 -0.306374
O8 -0.961236 2.685753 0.129257
N9 1.291827 -1.191315 -0.890191
N10 -3.236137 -1.304283 0.292104
H11 -4.064958 -0.789169 0.557722
H12 -3.290335 -2.308398 0.189467
N13 1.479610 0.992828 -0.704157
H14 1.548696 -2.166330 -0.997026
H15 -2.892519 1.152749 0.479192
H16 3.143224 -0.198435 -1.359393
O17 1.983499 -0.475904 1.696121
O18 2.922145 -0.327885 0.871720
H19 1.898237 1.915733 -0.648455

[8-OOG + H]$^+$ (open-shell)
O1 2.417625 -0.392384 1.592568
O2 3.098571 -0.284703 0.488401
C3 0.143359 0.667288 -0.316773
C4 0.033498 -0.753151 -0.406959
C5 -2.149430 -0.714956 0.080342
C6 -1.011091 1.454038 -0.000567
C7 2.213436 -0.169653 -0.705983
N8 -2.133112 0.647766 0.186597
N9 -1.062768 -1.452707 -0.223881
O10 -1.060431 2.675503 0.105219
N11 1.252146 -1.217006 -0.743530
N12 -3.293386 -1.336179 0.294237
H13 -4.139567 -0.831355 0.524111
H14 -3.324525 -2.344092 0.219637
N15 1.407057 1.010456 -0.607821
H16 1.510066 -2.193190 -0.823398
H17 -2.996103 1.133430 0.418597
H18 2.933840 -0.162293 -1.521043
H19 1.801976 1.942460 -0.546981

TS2$^+$ (open-shell)



C1 -0.773050 1.476505 -0.086254
C2 0.344098 0.598332 -0.391869
H3 -2.765617 1.287330 0.352078
C4 -2.042847 -0.618540 0.018525
H5 1.549794 -2.358304 -0.631142
C6 2.310167 -0.363881 -0.513011
N7 -1.933895 0.746198 0.124061
N8 1.581207 0.849653 -0.800128
N9 1.331215 -1.374112 -0.740279
N10 -1.008219 -1.443066 -0.260559
C11 0.134738 -0.835338 -0.442103
N12 -3.225908 -1.151585 0.218644
H13 -3.329238 -2.156436 0.156389
H14 -4.038678 -0.587214 0.435285
O15 -0.731969 2.691885 -0.017684
H16 3.267138 -0.480239 -1.006378
H17 2.027690 1.758935 -0.701252
O18 1.429628 -0.286840 1.602041
O19 2.582276 -0.204565 0.927033

endoperoxide
[5,8-OO-G + H]$^+$
C1 -0.607674 1.427409 -0.138858
C2 0.540053 0.449610 -0.090016
H3 -2.641326 1.435382 0.012682
C4 -2.050695 -0.546073 0.036635
H5 1.435068 -2.616626 -0.375415
C6 2.290454 -0.587844 -0.373790
N7 -1.834181 0.814476 -0.014024
N8 1.626172 0.529716 -1.014431
N9 1.267349 -1.619278 -0.452963
N10 -1.080312 -1.478859 -0.089549

C11 0.120876 -0.994254 -0.233078
N12 -3.283989 -0.952547 0.196830
H13 -3.472006 -1.947867 0.215420
H14 -4.056319 -0.303214 0.290119
O15 -0.468062 2.623719 -0.251825
H16 3.270942 -0.874074 -0.737406
H17 2.154727 1.391196 -0.869261
O18 1.144709 0.489236 1.234668
O19 2.409047 -0.192010 1.001840

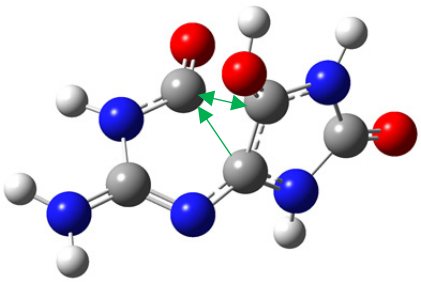
[8-H-8-OOHG + H]$^+$
C1 -1.092110 1.463476 -0.031274
C2 0.118203 0.646404 -0.294013
H3 -3.081675 1.158199 0.331875
C4 -2.223511 -0.708538 0.119352
C5 2.099040 -0.168320 -0.743235
N6 -2.206380 0.668967 0.155553
N7 1.308798 1.040555 -0.516070
N8 1.184461 -1.283675 -0.528950
N9 -1.141149 -1.484304 -0.103187
C10 -0.027092 -0.823575 -0.295227
N11 -3.376845 -1.296062 0.322592
H12 -3.421342 -2.307389 0.303857
H13 -4.224597 -0.770454 0.500055
O14 -1.126011 2.674075 0.017236
H15 2.470587 -0.161437 -1.771621
O16 2.878152 -0.230049 1.414001
O17 3.250418 -0.230290 0.035769
H18 3.162546 0.653718 1.698858
H19 1.444637 -2.257569 -0.642252

[8-OOHG + H]$^+$
C1 1.071520 1.450393 -0.000695
C2 -0.009337 0.533492 -0.000171
H3 3.117431 1.349577 0.000996
C4 2.440006 -0.601171 0.003336
H5 -1.197014 -2.437686 -0.004944
C6 -1.945516 -0.479356 -0.003734
N7 2.286987 0.763214 0.001098
N8 -1.391566 0.718459 -0.001733
N9 -1.008374 -1.439538 -0.003951
N10 1.412336 -1.443760 0.002518
C11 0.231090 -0.820099 0.000203
N12 3.688169 -1.074641 0.006960
H13 3.832571 -2.073481 0.004986
H14 4.488184 -0.458568 0.003054
O15 1.030925 2.683845 -0.002591
H16 -4.418889 0.419761 0.788873
H17 -1.900974 1.596407 -0.007802
O18 -3.232297 -0.786611 -0.011298
O19 -3.993723 0.407553 -0.087741

[OG^{ox} + H]$^+$
C1 0.764410 1.464795 0.000001
C2 -0.467291 0.633952 0.000000
H3 2.795225 1.179079 0.000002
C4 1.931166 -0.688521 0.000001
C5 -2.447374 -0.235348 -0.000001
N6 1.906416 0.679662 0.000001
N7 -1.687021 1.004111 -0.000001
N8 -1.557375 -1.315701 -0.000001
N9 0.813479 -1.483713 0.000001
C10 -0.303472 -0.841987 0.000000
N11 3.085347 -1.289419 0.000001
H12 3.111137 -2.303305 0.000001
H13 3.961364 -0.775915 0.000001
O14 0.792020 2.672738 0.000001
O15 -3.643867 -0.294222 -0.000002
H16 -1.843500 -2.289918 0.000000

[5-OHOG + H]$^+$
C1 -0.732826 1.349219 -0.327642
C2 0.382740 0.558064 0.354130
H3 -2.758455 1.157871 -0.628629
C4 -2.020388 -0.700370 -0.109909
H5 1.623894 -2.397926 -0.365184
C6 2.387161 -0.401615 -0.225763
N7 -1.919377 0.640893 -0.372248
N8 1.714692 0.784320 -0.113656
N9 1.417912 -1.431417 -0.130304
N10 -0.937657 -1.521768 -0.035134
C11 0.202854 -0.917615 0.044711
N12 -3.209136 -1.230032 -0.015727
H13 -3.294975 -2.230320 0.122119
H14 -4.051519 -0.670432 -0.092054
O15 -0.635883 2.498971 -0.689814
H16 2.216150 1.635866 0.112413
H17 0.299959 1.629401 1.983250
O18 0.214100 0.694659 1.743053
O19 3.569615 -0.586697 -0.412687

TS3a$^+$

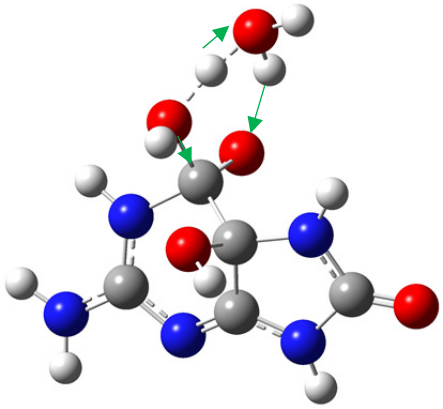


C1 0.520029 0.476787 0.872957
C2 0.047456 -0.727115 0.280312
C3 -2.122465 -0.478248 -0.066875
C4 -0.404816 0.921915 -0.794439
C5 2.274324 -0.549568 -0.113369
N6 -1.733081 0.679051 -0.740148
N7 -1.186065 -1.265364 0.403600
O8 0.229101 1.647699 -1.501090
N9 1.141031 -1.340088 -0.264072
N10 -3.414347 -0.739243 0.017747
H11 -4.104716 -0.107506 -0.364006
H12 -3.719790 -1.579163 0.489889
O13 3.382963 -0.763416 -0.560564
N14 1.866727 0.538481 0.643580
H15 1.093409 -2.105651 -0.928026
O16 -0.134859 1.147975 1.801174
H17 2.457848 1.343518 0.821799
H18 -2.373987 1.175862 -1.355472
H19 0.222580 2.042403 1.923195

[Sp + H]$^+$
C1 -0.814323 1.081298 0.370793
C2 0.000773 -0.049908 -0.229280
C3 2.164281 0.032820 -0.537656
C4 0.704005 -0.846914 0.920404
C5 -2.288773 -0.358539 -0.555009
N6 2.020289 -0.704490 0.639769
N7 1.043962 0.412453 -1.093357
O8 0.167238 -1.446893 1.826863
N9 -1.055709 -0.815464 -0.847016
N10 3.384440 0.289429 -0.991785
H11 4.200645 -0.088200 -0.532525
H12 3.495788 0.802122 -1.854507
O13 -3.381268 -0.799172 -0.827571
N14 -2.087006 0.862074 0.185462
H15 -0.905533 -1.736680 -1.239887
O16 -0.237700 2.057256 0.951558
H17 -2.853575 1.461142 0.488114
H18 2.777144 -1.129903 1.164322
H19 -0.838237 2.741440 1.300647

[5-OHOG·2H$_2$O + H]$^+$
C1 0.825658 -0.524281 -0.106460
C2 1.143077 0.963972 -0.163734
C3 -1.000107 1.478133 0.183271
C4 -0.329046 -0.733316 0.874443
C5 3.095740 -0.157363 0.041873
N6 -1.229925 0.312967 0.860998
N7 0.250793 1.899274 -0.160293
O8 -0.500277 -1.747663 1.510642
N9 2.468522 1.087575 -0.212794
N10 -2.009697 2.270696 -0.056941
H11 -2.957567 2.011788 0.194902
H12 -1.844595 3.164862 -0.503322
O13 4.295080 -0.324109 0.095764
N14 2.097767 -1.067051 0.246902
H15 2.983094 1.962876 -0.240584
O16 0.288708 -1.000613 -1.315221
H17 0.858656 -0.757065 -2.060873
H18 2.283486 -2.062781 0.220537
H19 -2.215970 0.069998 1.099947
O20 -3.822399 -0.551501 0.772190
H21 -4.448596 0.176506 0.683192
H22 -2.910508 -2.079756 -1.970126
O23 -2.742344 -1.161439 -1.728746
H24 -1.777058 -1.090776 -1.678127
H25 -3.575246 -0.800150 -0.144033

TS3b$^+$ PCM-B3LYP/6-31+G(d,p)

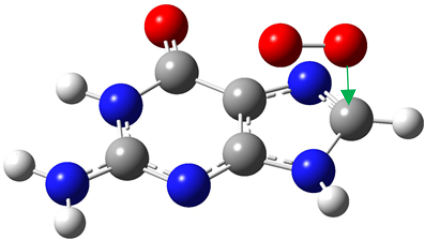


C1 -0.407953 0.031739 0.565252
C2 -0.289858 1.421532 -0.077902
C3 1.959787 1.267554 -0.203564
C4 0.648947 -0.857490 -0.179640
C5 -2.491563 0.816497 -0.144722
N6 1.924941 -0.062463 -0.090376
N7 0.820953 2.031246 -0.332770
O8 0.342468 -1.290140 -1.340167
N9 -1.534135 1.852413 -0.341946
N10 3.109821 1.930555 -0.248478
H11 4.007932 1.471604 -0.189833
H12 3.084959 2.935570 -0.353120
O13 -3.677300 0.911445 -0.385242
N14 -1.790622 -0.257913 0.335958
H15 -1.769574 2.726130 -0.799422
O16 -0.038853 0.038692 1.931331
H17 -0.716029 0.484378 2.464666
H18 -2.247939 -1.120328 0.600425
H19 2.783590 -0.599441 -0.146783

O20 0.978275 -2.044018 0.772590
H21 0.750292 -1.815134 1.695035
H22 -0.122090 -2.915884 -1.229548
O23 -0.042921 -3.696499 -0.595074
H24 -0.926814 -4.044134 -0.393010
H25 0.429457 -3.014451 0.270832

[*gem*-diol + H]$^+$
C1 0.407885 0.423664 0.453331
C2 0.324127 -1.037859 0.011955
C3 -1.917241 -0.964769 -0.050480
C4 -0.705347 1.174270 -0.309840
C5 2.490697 -0.395042 -0.121229
N6 -1.920396 0.370152 -0.124229
N7 -0.765902 -1.709919 -0.141134
N8 1.574947 -1.467218 -0.184070
N9 -3.046808 -1.628353 0.072639
H10 -3.940038 -1.154200 0.113251
H11 -3.019058 -2.637887 0.121892
O12 3.690359 -0.503837 -0.279140
N13 1.764113 0.735975 0.111483
H14 1.840351 -2.396770 -0.492750
O15 0.104797 0.591415 1.808303
H16 0.720026 0.083557 2.356266
H17 2.213781 1.581954 0.440503
O18 -0.327363 1.246360 -1.634947
H19 -1.047054 1.635224 -2.152185
H20 -1.038627 2.422740 1.135693
O21 -0.939083 2.451683 0.171963
H22 -2.801467 0.874369 -0.097345

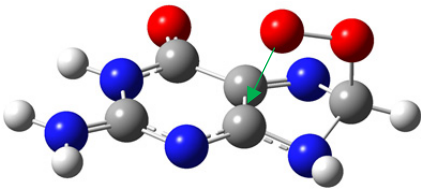
TS1 (open-shell)



C1 0.386652 0.651761 -0.417595
C2 0.188662 -0.763780 -0.490316
C3 -1.978563 -0.654439 0.002747
C4 -0.756045 1.481561 -0.088307
C5 2.282208 -0.203185 -0.762871
N6 -1.897846 0.716076 0.120059
N7 -0.947933 -1.435022 -0.318764
O8 -0.782497 2.703070 0.009493
N9 1.385099 -1.252765 -0.872945
N10 -3.164275 -1.204792 0.231868
H11 -3.974989 -0.649595 0.468303
H12 -3.258535 -2.208031 0.162802
N13 1.636932 0.993313 -0.705821
H14 1.647611 -2.230983 -0.861512
H15 -2.738016 1.232124 0.367633
H16 3.297878 -0.311590 -1.110626
O17 1.381259 -0.401821 1.653143
O18 2.551830 -0.253887 1.128699

8-OOG
C1 -1.075751 1.460217 -0.014974
C2 0.148020 0.660620 -0.259616
H3 -3.067574 1.131250 0.310908
C4 -2.185850 -0.726048 0.099339
H5 1.499314 -2.225890 -0.624013
C6 2.160590 -0.122939 -0.689434
N7 -2.185132 0.653096 0.142584
N8 1.340717 1.071255 -0.434058
N9 1.225411 -1.253530 -0.538903
N10 -1.100492 -1.485843 -0.131304
C11 0.015792 -0.809141 -0.301436
N12 -3.338427 -1.322150 0.302271
H13 -3.376632 -2.333120 0.280735
H14 -4.186932 -0.802245 0.489179
O15 -1.128298 2.671356 0.043082
H16 2.494562 -0.069953 -1.731106
O17 2.926172 -0.224529 1.489743
O18 3.285365 -0.211339 0.078036

TS, to endoperoxide



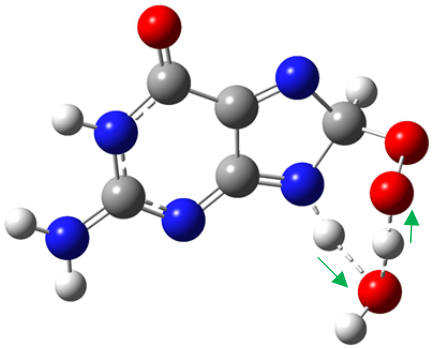
C1 -0.825218 1.502259 -0.040689
C2 0.402643 0.736054 -0.333950
C3 -1.908661 -0.706907 -0.037362
H4 1.764633 -2.081927 -0.839273
C5 2.352872 -0.092120 -0.455205
N6 -1.916441 0.670802 0.110460
N7 1.599882 1.153542 -0.530192
N8 1.471183 -1.117633 -0.967400
N9 -0.833652 -1.431816 -0.343592
C10 0.294906 -0.731027 -0.410709
N11 -3.069955 -1.312061 0.134940
H12 -3.113388 -2.317739 0.042201
H13 -3.918019 -0.800480 0.338924

O14 -0.905022 2.712320 0.065885
H15 3.348843 -0.066404 -0.879023
O16 1.181378 -0.602694 1.446953
O17 2.481095 -0.341005 0.967965
H18 -2.798054 1.128202 0.328731

endoperoxide
4,8-OO-G
C1 -0.882959 1.511976 0.029796
C2 0.396362 0.806448 -0.202528
C3 -1.841000 -0.758151 -0.051356
H4 1.896891 -1.858896 -0.993946
C5 2.357163 0.040132 -0.433404
N6 -1.928127 0.633179 0.112364
N7 1.566073 1.286935 -0.387041
N8 1.512271 -0.919271 -1.094164
N9 -0.737922 -1.433177 -0.226774
C10 0.435545 -0.691309 -0.163496
N11 -3.023535 -1.379697 -0.021330
H12 -3.047276 -2.382057 -0.136988
H13 -3.893817 -0.872167 0.044972
O14 -1.016824 2.721841 0.125775
H15 3.371642 0.150592 -0.797639
O16 2.425541 -0.412168 0.940441
O17 1.091978 -0.916219 1.167231
H18 -2.844997 1.044532 0.260567

8-OOG·H_2O
C1 1.649586 -1.341288 0.352003
C2 0.320402 -0.979288 -0.197619
C3 2.198517 1.011932 -0.083561
C4 -1.754506 -0.864313 -0.922314
N5 2.509691 -0.260871 0.347490
N6 -0.713627 -1.711870 -0.323067
N7 -1.112132 0.444372 -1.105514
N8 1.010171 1.377694 -0.599408
C9 0.117288 0.412752 -0.650793
N10 3.142381 1.918536 0.022549
H11 2.952599 2.864261 -0.283664
H12 4.052324 1.702373 0.411877
O13 1.973544 -2.436243 0.762575
H14 -2.021264 -1.285978 -1.895454
O15 -2.911254 -0.812416 -0.184988
O16 -2.621926 -0.294983 1.138817
O17 -2.835773 2.307851 0.945664
H18 -2.738902 1.307389 0.998025
H19 -1.949699 2.640993 0.769721
H20 -1.617268 1.274505 -1.395654
H21 3.442371 -0.431023 0.717962

TS2



C1 1.749290 -1.343123 0.178441
C2 0.370930 -0.969574 -0.220209
C3 2.183631 1.066212 -0.001722
C4 -1.739271 -0.830613 -0.771843
N5 2.568795 -0.235502 0.252980
N6 -0.664940 -1.709145 -0.288977
N7 -1.174732 0.511983 -0.873059
N8 0.954573 1.437646 -0.397220
C9 0.089679 0.449457 -0.516643
N10 3.101227 1.993784 0.156366
H11 2.857691 2.959509 -0.022811
H12 4.043737 1.771705 0.453333
O13 2.139670 -2.467886 0.416133
H14 -2.035313 -1.206946 -1.755882
O15 -2.901520 -0.867545 -0.011403
O16 -2.689754 -0.208717 1.249303
O17 -2.890698 2.015919 0.306305
H18 -2.825368 0.878274 0.919459
H19 -2.432014 2.670857 0.844527
H20 -1.825304 1.337027 -0.600877
H21 3.534973 -0.410127 0.520780

8-H-8-OOHG
C1 -1.087347 1.450005 -0.009543
C2 0.127094 0.643366 -0.273833
C3 -2.193355 -0.742862 0.102516
C4 2.057060 -0.193289 -0.735847
N5 -2.189747 0.651441 0.160951
N6 1.320106 1.053818 -0.461643
N7 1.194216 -1.339316 -0.549293
N8 -1.139818 -1.497051 -0.132013
C9 0.026603 -0.832183 -0.320360
N10 -3.380694 -1.304497 0.308995
H11 -3.451012 -2.311779 0.292705
H12 -4.205724 -0.757897 0.512012
O13 -1.132297 2.667083 0.052934
H14 2.382243 -0.141142 -1.780986
O15 2.982489 -0.329303 1.367613

O16 3.266499 -0.261242 -0.031716
H17 3.202004 0.568397 1.663455
H18 -3.069804 1.129108 0.335596

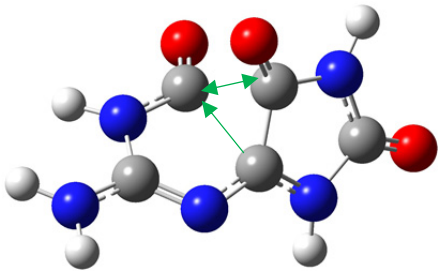
8-OOHG
C1 -1.195532 1.429228 0.018021
C2 -0.001590 0.664357 -0.107916
C3 -2.314741 -0.767530 0.067703
H4 1.498710 -2.128793 -0.312726
C5 1.968787 -0.049952 -0.308123
N6 -2.320331 0.605045 0.101510
N7 1.314550 1.070824 -0.216919
N8 1.178878 -1.169194 -0.261987
N9 -1.211691 -1.483636 -0.046044
C10 -0.101689 -0.722491 -0.130092
N11 -3.514857 -1.375702 0.121088
H12 -3.519354 -2.372584 0.281544
H13 -4.329152 -0.854656 0.414517
O14 -1.324035 2.660587 0.060431
H15 4.158422 0.505044 1.088651
O16 3.308795 -0.151447 -0.476916
O17 3.908476 -0.394925 0.819127
H18 -3.211775 1.084242 0.185786

OG^{ox}
C1 0.828413 1.442115 0.000000
C2 -0.425724 0.628532 0.000000
C3 1.958986 -0.597871 0.000001
C4 -2.410691 -0.242005 -0.000001
N5 1.982049 0.738168 0.000001
N6 -1.650858 0.992393 -0.000001
N7 -1.532901 -1.321300 -0.000001
N8 0.851362 -1.466788 0.000000
C9 -0.266964 -0.843894 0.000000
N10 3.111157 -1.238798 0.000001
H11 3.131675 -2.249508 0.000001
H12 3.979363 -0.719734 0.000002
O13 0.773907 2.673022 0.000000
O14 -3.613673 -0.296167 -0.000001
H15 -1.822690 -2.292589 -0.000001

5-OHOG
C1 -0.796339 1.331257 -0.337386
C2 0.337508 0.556763 0.345621
C3 -2.043288 -0.609793 -0.145586
C4 2.349075 -0.408135 -0.210888
N5 -1.992538 0.704500 -0.396830
N6 1.671211 0.777868 -0.119556
N7 1.399299 -1.439233 -0.103261
N8 -0.968859 -1.502876 -0.110436
C9 0.164912 -0.917925 0.030351
N10 -3.225945 -1.181215 -0.005190
H11 -3.294592 -2.180466 0.127911
H12 -4.068823 -0.625377 -0.051284
O13 -0.607577 2.491301 -0.708152
H14 2.169667 1.626122 0.121788
H15 -0.601166 0.799788 2.073087
O16 0.307959 0.779799 1.742474
O17 3.540812 -0.577006 -0.392521
H18 1.611985 -2.399131 -0.351672

5-OHOG_2
C1 -0.732526 1.358648 -0.277733
C2 0.379619 0.582415 0.416539
C3 -2.007286 -0.707381 -0.102301
C4 2.389537 -0.378230 -0.219407
N5 -1.918477 0.635036 -0.347314
N6 1.727220 0.804433 -0.121792
N7 1.424808 -1.411411 -0.113485
N8 -0.925767 -1.521738 -0.010890
C9 0.211512 -0.892969 0.064844
N10 -3.199973 -1.247186 -0.033935
H11 -3.281288 -2.247706 0.095617
H12 -4.043024 -0.693043 -0.124832
O13 -0.685423 2.528158 -0.607447
H14 2.247723 1.622876 0.172159
O15 0.232565 0.796853 1.739258
O16 3.578462 -0.580000 -0.399351
H17 1.637742 -2.380673 -0.326239
H18 -2.765792 1.149609 -0.576128

TS3a



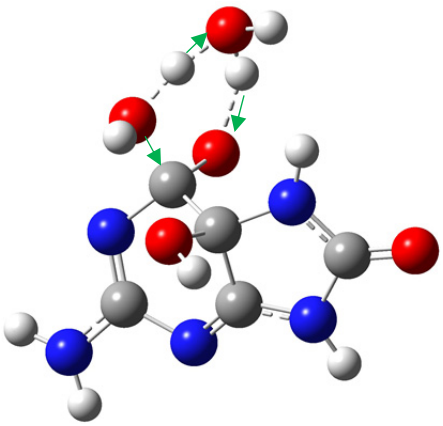
C1 0.486780 0.407022 0.921610
C2 0.091857 -0.801970 0.209017
C3 -2.091686 -0.510654 -0.100458
C4 -0.450428 1.101890 -0.603831
C5 2.304842 -0.501028 -0.163611
N6 -1.767948 0.747787 -0.584004
N7 -1.131407 -1.353870 0.200329
O8 0.027820 2.061037 -1.159287
N9 1.196241 -1.325980 -0.380718
N10 -3.377052 -0.829845 -0.024255

H11 -4.095548 -0.185519 -0.323205
H12 -3.637171 -1.763916 0.259585
O13 3.417815 -0.672014 -0.641501
N14 1.874215 0.502082 0.650020
O15 -0.076759 0.989143 1.890287
H16 2.457360 1.280280 0.928164
H17 -2.462795 1.311697 -1.067388
H18 1.180612 -2.020655 -1.119109

Sp
C1 0.796286 -1.038377 0.637648
C2 0.001783 -0.026231 -0.219938
C3 -2.167954 -0.153755 -0.507498
C4 -0.688654 0.983473 0.733740
C5 2.293007 0.186564 -0.583892
N6 -2.011461 0.799309 0.503574
N7 -1.056979 -0.642357 -0.977152
O8 -0.154445 1.752369 1.512177
N9 1.059707 0.576096 -0.994748
N10 -3.397730 -0.468791 -0.912272
H11 -4.212477 -0.066002 -0.473808
H12 -3.516389 -1.177478 -1.620884
O13 3.376792 0.602089 -0.966843
N14 2.110781 -0.820529 0.368823
H15 0.936921 1.445026 -1.499085
O16 0.319426 -1.854272 1.402581
H17 2.881363 -1.333973 0.781035
H18 -2.760637 1.314814 0.951486

5-OHOG·2H2O
C1 0.006679 -0.100458 0.204124
C2 -1.174438 -1.051050 0.093773
C3 -2.538201 0.708801 -0.064635
C4 -0.338287 1.165491 -0.593011
C5 0.708344 -2.252197 -0.247373
N6 -1.620661 1.563807 -0.535298
N7 -2.400486 -0.674276 0.064115
O8 0.550537 1.799290 -1.171913
N9 -0.676674 -2.297777 0.000870
N10 -3.742672 1.168823 0.215332
H11 -3.943116 2.154960 0.118012
H12 -4.471292 0.537509 0.519017
O13 1.410748 -3.227786 -0.437753
N14 1.069281 -0.935232 -0.273208
H15 -1.222015 -3.142494 -0.131495
O16 0.188060 0.358684 1.526131
H17 0.281055 -0.394926 2.128825
H18 2.041412 -0.661133 -0.194408
H19 3.196505 1.370183 0.788347
O20 2.998605 1.300241 1.742638
H21 2.059234 1.064863 1.767499
H22 2.348216 1.574593 -1.164957
O23 3.318312 1.544505 -1.044241
H24 3.593807 0.696029 -1.409691

TS3b

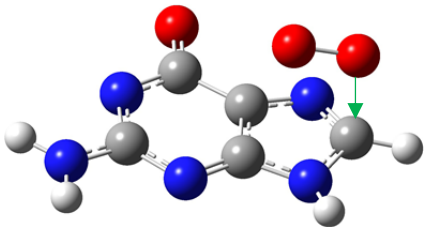


C1 -0.280533 0.096288 0.556924
C2 0.205118 1.386443 -0.086892
C3 2.267479 0.497236 -0.215349
C4 0.491936 -1.028394 -0.187785
C5 -2.058988 1.433269 -0.097432
N6 1.906658 -0.744204 -0.135856
N7 1.422714 1.623079 -0.396876
O8 0.014174 -1.297172 -1.388068
N9 -0.882159 2.169994 -0.294529
N10 3.574800 0.844813 -0.158587
H11 4.267716 0.113289 -0.219160
H12 3.837925 1.769363 -0.464643
O13 -3.187712 1.854185 -0.307779
N14 -1.693769 0.200919 0.339197
H15 -0.880955 3.065777 -0.767615
O16 0.065620 0.022089 1.920956
H17 -0.345884 0.749691 2.407109
H18 -2.365188 -0.515269 0.580982
H19 -0.687020 -2.799465 0.251395
O20 0.316375 -2.275462 0.678588
H21 0.258126 -2.026454 1.616455
H22 -1.145887 -2.348073 -1.168402
O23 -1.531626 -3.078544 -0.562052
H24 -2.401268 -2.780876 -0.259511

***gem*-diol**
C1 0.373340 0.418741 0.454701
C2 0.298488 -1.036955 0.014244
C3 -1.942648 -0.869685 -0.051935
C4 -0.762896 1.140204 -0.298079
C5 2.463866 -0.390641 -0.120782

N6 -2.000650 0.429567 -0.126624
N7 -0.790513 -1.681667 -0.171731
N8 1.568888 -1.468027 -0.163999
N9 -3.062337 -1.593728 0.123087
H10 -3.961145 -1.136074 0.103378
H11 -3.020282 -2.597029 0.033445
O12 3.670537 -0.482349 -0.285223
N13 1.732343 0.737829 0.105265
H14 1.840036 -2.386285 -0.495132
O15 0.104920 0.578709 1.824308
H16 2.179381 1.587375 0.425952
O17 -0.366865 1.204925 -1.639932
H18 -1.159009 1.381089 -2.165474
H19 -1.366609 2.453244 0.998522
O20 -0.901930 2.463635 0.151657
H21 0.719313 0.040508 2.341947

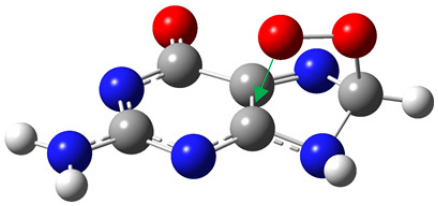
TS1^{-} (open-shell)



C1 0.350808 0.638732 -0.420639
C2 0.147263 -0.773401 -0.496176
C3 -1.999528 -0.562257 0.018683
C4 -0.809157 1.458259 -0.081864
C5 2.238899 -0.218929 -0.825510
N6 -1.963193 0.781917 0.139636
N7 -0.992242 -1.416528 -0.309806
O8 -0.743392 2.706779 0.002477
N9 1.348763 -1.271924 -0.882300
N10 -3.188703 -1.143680 0.253463
H11 -3.985493 -0.581983 0.508752
H12 -3.280366 -2.145965 0.198135
N13 1.605128 0.970398 -0.735337
H14 1.613737 -2.248271 -0.873884
H15 3.257597 -0.336078 -1.161915
O16 1.349835 -0.351953 1.676190
O17 2.538126 -0.277752 1.184128

[8-OOG – H]$^{-}$
C1 -1.142157 1.435347 -0.002089
C2 0.105624 0.659101 -0.257736
C3 -2.208979 -0.641171 0.110089
C4 2.124126 -0.121291 -0.694524
N5 -2.261922 0.706215 0.171631
N6 1.300396 1.068607 -0.437831
N7 1.199139 -1.253624 -0.562185
N8 -1.133734 -1.467494 -0.135758
C9 -0.019458 -0.810243 -0.308948
N10 -3.354030 -1.281768 0.315827
H11 -3.382706 -2.290587 0.290269
H12 -4.195740 -0.760199 0.512539
O13 -1.117682 2.673752 0.043315
H14 2.484895 -0.057707 -1.726168
O15 3.250518 -0.208330 0.087102
O16 2.893574 -0.240846 1.498567
H17 1.478404 -2.222122 -0.651056

TS^{-}, to endoperoxide



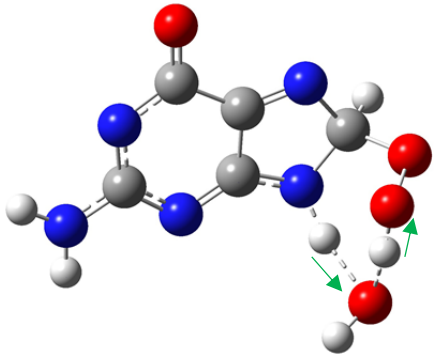
C1 -0.906039 1.479013 -0.009192
C2 0.358656 0.753320 -0.301251
C3 -1.917879 -0.635553 -0.033018
C4 2.325368 -0.052303 -0.445430
N5 -2.000763 0.713072 0.138123
N6 1.554241 1.187370 -0.480258
N7 1.462546 -1.067487 -1.010601
N8 -0.846166 -1.407015 -0.350197
C9 0.285591 -0.716011 -0.382659
N10 -3.072096 -1.291032 0.119098
H11 -3.104543 -2.292285 0.001382
H12 -3.918101 -0.780468 0.320034
O13 -0.916507 2.720261 0.094354
H14 3.324579 0.009513 -0.859895
O15 1.136080 -0.698922 1.384204
O16 2.450772 -0.375025 0.960923
H17 1.776788 -2.022431 -0.861217

endoperoxide
[4,8-OO-G – H]$^{-}$
C1 -0.944297 1.483431 0.040318
C2 0.356197 0.800713 -0.199253
C3 -1.869158 -0.678015 -0.043294
H4 1.864832 -1.864903 -0.987086
C5 2.325271 0.040752 -0.443571
N6 -2.010439 0.686106 0.117761
N7 1.529093 1.278793 -0.392911
N8 1.479275 -0.926932 -1.095681
N9 -0.779015 -1.417359 -0.216531

C10 0.395208 -0.693803 -0.168320
N11 -3.048959 -1.329833 -0.030922
H12 -3.070258 -2.335980 -0.083099
H13 -3.902044 -0.817081 0.123354
O14 -0.993341 2.730060 0.145724
H15 3.336662 0.152684 -0.817283
O16 2.413580 -0.420725 0.929866
O17 1.079985 -0.920410 1.171512

[8-OOG·H_2O – H]$^-$
C1 -1.712867 -1.288849 -0.356935
C2 -0.356140 -0.991746 0.190270
C3 -2.187018 0.961432 0.061578
C4 1.736961 -0.923927 0.883840
N5 -2.570027 -0.249844 -0.389901
N6 0.671643 -1.741041 0.287974
N7 1.109645 0.365651 1.173941
N8 -0.994242 1.346600 0.640143
C9 -0.122239 0.379188 0.688266
N10 -3.078158 1.937942 -0.052177
H11 -2.851728 2.871693 0.258119
H12 -3.975695 1.754039 -0.476356
O13 -2.003947 -2.427226 -0.750483
H14 2.077895 -1.404264 1.803953
O15 2.858095 -0.822748 0.078952
O16 2.506381 -0.219587 -1.190789
O17 2.703905 2.361660 -0.877490
H18 2.615466 1.360290 -0.969717
H19 1.849581 2.664241 -0.552006
H20 1.644782 1.185469 1.432506

TS2$^-$



C1 1.809355 -1.291218 0.188810
C2 0.411335 -0.960500 -0.214335
C3 2.210530 1.004877 0.021983
C4 -1.703835 -0.845945 -0.773336
N5 2.648643 -0.243385 0.290757
N6 -0.620543 -1.708997 -0.288122
N7 -1.160817 0.497612 -0.906807
N8 0.970044 1.427047 -0.404589
C9 0.111948 0.450451 -0.526850
N10 3.097289 1.980931 0.177569
H11 2.837279 2.938046 -0.011512
H12 4.035020 1.767404 0.484848
O13 2.147079 -2.463564 0.409595
H14 -2.034938 -1.244374 -1.736386
O15 -2.857795 -0.882372 0.016905
O16 -2.620915 -0.222120 1.267590
O17 -2.853210 2.055746 0.286665
H18 -2.760501 0.791786 0.973300
H19 -2.367094 2.716395 0.792452
H20 -1.809335 1.310766 -0.608030

[8-H-8-OOHG – H]$^-$
C1 -1.148292 1.425407 -0.001149
C2 0.087545 0.638927 -0.275503
C3 -2.215517 -0.656975 0.113186
C4 2.021313 -0.203772 -0.741789
N5 -2.264830 0.709785 0.181717
N6 1.284596 1.042550 -0.469631
N7 1.162719 -1.349838 -0.558762
N8 -1.176850 -1.477177 -0.127184
C9 -0.010270 -0.837184 -0.322019
N10 -3.397218 -1.256617 0.322950
H11 -3.461298 -2.262857 0.311052
H12 -4.214447 -0.704328 0.530102
O13 -1.111433 2.672415 0.051717
H14 2.369261 -0.150318 -1.779507
O15 2.944774 -0.324130 1.374061
O16 3.230767 -0.266755 -0.025556
H17 3.126032 0.585916 1.656596

[8-OOHG – H]$^-$
C1 1.254187 1.405318 -0.020399
C2 0.042131 0.654162 0.112690
C3 2.345530 -0.677453 -0.071833
H4 -1.464394 -2.144371 0.312654
C5 -1.933915 -0.067884 0.312266
N6 2.398789 0.667095 -0.114821
N7 -1.280578 1.054922 0.222464
N8 -1.144022 -1.185952 0.264057
N9 1.263033 -1.463046 0.048106
C10 0.141787 -0.730765 0.132997
N11 3.558587 -1.324524 -0.112887
H12 3.527996 -2.295999 -0.388322
H13 4.321841 -0.793630 -0.507200
O14 1.291124 2.671899 -0.057841
H15 -4.120424 0.529147 -1.076581
O16 -3.276457 -0.171700 0.475895

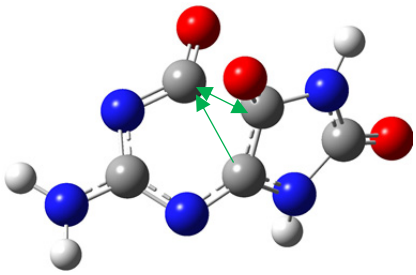
O17 -3.881418 -0.379559 -0.828468

[OG^{ox} – H]$^-$
C1 0.793825 1.431286 0.000000
C2 -0.452829 0.611841 0.000000
C3 1.913988 -0.613625 0.000001
C4 -2.387216 -0.337740 -0.000001
N5 1.946752 0.737331 0.000000
N6 -1.678190 0.966436 -0.000001
N7 -1.541028 -1.417777 0.000000
N8 0.837324 -1.476128 0.000001
C9 -0.325600 -0.875642 0.000000
N10 3.094029 -1.221204 0.000001
H11 3.145108 -2.229575 0.000001
H12 3.943542 -0.675071 0.000001
O13 0.738180 2.670008 -0.000001
O14 -3.607414 -0.359092 -0.000001

[5-OHOG – H]$^-$
C1 -0.761024 1.324814 -0.328136
C2 0.368089 0.530263 0.329594
C3 -2.006104 -0.618819 -0.135818
C4 2.316899 -0.492416 -0.224518
N5 -1.953755 0.709735 -0.404186
N6 1.699578 0.748896 -0.124374
N7 1.386627 -1.523329 -0.219246
N8 -0.973133 -1.509750 -0.070613
C9 0.218548 -0.945876 -0.008733
N10 -3.223679 -1.144169 -0.005563
H11 -3.332481 -2.136085 0.145070
H12 -4.040998 -0.559353 -0.095675
O13 -0.569191 2.500299 -0.678211
H14 2.229001 1.535034 0.231700
H15 -0.561291 0.573156 2.081092
O16 0.327493 0.741578 1.738646
O17 3.533931 -0.638155 -0.359018

[5-OHOG – H]$^-$_2
C1 -0.790239 1.336242 -0.289825
C2 0.327659 0.570193 0.417241
C3 -2.034556 -0.605996 -0.136046
C4 2.351860 -0.384078 -0.202268
N5 -1.993328 0.707681 -0.373453
N6 1.686172 0.796561 -0.111756
N7 1.402560 -1.418023 -0.102906
N8 -0.961324 -1.496132 -0.101334
C9 0.169726 -0.895360 0.045550
N10 -3.221507 -1.186832 -0.007606
H11 -3.285777 -2.186621 0.116106
H12 -4.065600 -0.634511 -0.053030
O13 -0.634334 2.515190 -0.637863
H14 2.202154 1.616198 0.184604
O15 0.208102 0.761690 1.758585
O16 3.550790 -0.572786 -0.373828
H17 1.618040 -2.376594 -0.351355

TS3a$^-$



C1 0.436220 0.449534 0.887774
C2 0.047147 -0.801895 0.303625
C3 -2.093993 -0.440422 -0.139745
C4 -0.503001 1.084601 -0.659236
C5 2.251411 -0.530367 -0.141326
N6 -1.777471 0.751011 -0.737148
N7 -1.190594 -1.317296 0.289609
O8 0.121225 1.991015 -1.192099
N9 1.154144 -1.372879 -0.273171
N10 -3.395570 -0.745468 -0.071283
H11 -4.078633 -0.113307 -0.458016
H12 -3.689552 -1.636825 0.297544
O13 3.360259 -0.715937 -0.646198
N14 1.839228 0.510224 0.628438
O15 -0.104640 1.119101 1.841360
H16 2.398334 1.342529 0.758238
H17 1.120235 -2.093689 -0.983945

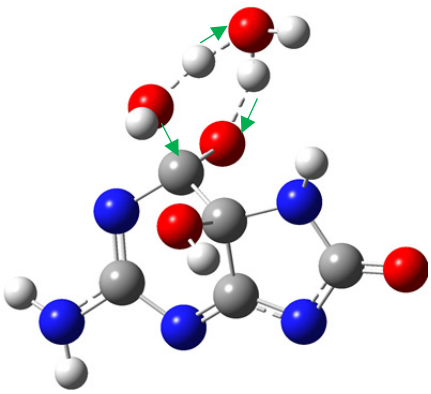
[Sp – H]$^-$
C1 0.746531 1.141140 -0.423948
C2 -0.038216 0.003375 0.239645
C3 -2.190952 -0.003801 0.436343
C4 -0.721749 -0.849222 -0.876254
C5 2.254117 -0.278204 0.542194
N6 -2.038419 -0.782663 -0.699764
N7 -1.123632 0.457225 1.057782
O8 -0.079896 -1.455932 -1.755220
N9 1.027269 -0.710802 0.918362
N10 -3.446177 0.273004 0.848239
H11 -4.203342 -0.276873 0.472109
H12 -3.574880 0.678678 1.762977
O13 3.345407 -0.765287 0.817695
N14 2.067793 0.874525 -0.224571
O15 0.275593 2.090630 -1.028128
H16 2.835138 1.448681 -0.552790

H17 0.908024 -1.664530 1.234707

[5-OHOG·2H$_2$O – H]$^-$

C1 -0.012654 0.112499 0.164701
C2 1.105197 1.143405 0.046644
C3 2.562344 -0.567518 -0.020643
C4 0.399151 -1.160416 -0.574628
C5 -0.737072 2.219268 -0.300132
N6 1.692500 -1.489259 -0.507737
N7 2.369850 0.774805 0.121547
O8 -0.459558 -1.867877 -1.134841
N9 0.634675 2.364445 -0.118265
N10 3.785940 -1.009102 0.259399
H11 4.013561 -1.984073 0.131752
H12 4.492260 -0.365590 0.584822
O13 -1.532409 3.148151 -0.454828
N14 -1.100335 0.882195 -0.347129
O15 -0.192273 -0.310690 1.510323
H16 -0.243805 0.467591 2.084249
H17 -2.059106 0.608373 -0.168992
H18 -3.151564 -1.345842 0.819106
O19 -2.975531 -1.162559 1.762842
H20 -2.034845 -0.923993 1.777621
H21 -2.222799 -1.684360 -1.090879
O22 -3.199403 -1.686795 -0.991657
H23 -3.500516 -0.878978 -1.422744

TS3b$^-$



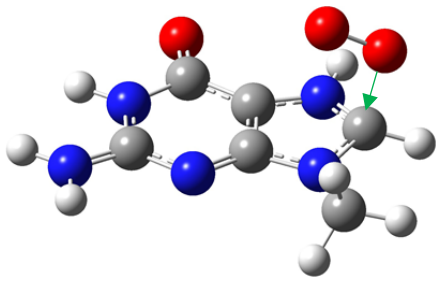
C1 0.330967 -0.105122 0.479085
C2 -0.097098 -1.425879 -0.162095
C3 -2.216221 -0.615042 -0.180077
C4 -0.533959 1.002758 -0.166307
C5 2.068728 -1.444514 -0.152339
N6 -1.922633 0.651780 -0.079525
N7 -1.355302 -1.693293 -0.389491
O8 -0.124143 1.385595 -1.371423
N9 0.953254 -2.206743 -0.423867
N10 -3.525218 -0.995413 -0.098077
H11 -4.223630 -0.275893 -0.215290
H12 -3.756177 -1.909201 -0.458444
O13 3.242273 -1.835318 -0.238606
N14 1.730698 -0.143245 0.191066
O15 0.053697 -0.085848 1.871051
H16 0.531857 -0.806966 2.300956
H17 2.383032 0.431422 0.708545
H18 0.562919 2.810379 0.316494
O19 -0.382023 2.226944 0.765140
H20 -0.241120 1.917052 1.675997
H21 0.911734 2.397255 -1.137450
O22 1.348408 3.157353 -0.549126
H23 2.245598 2.881327 -0.317443

[*gem*-diol – H]$^-$

C1 0.406672 0.395868 0.422758
C2 0.354775 -1.058325 -0.043799
C3 -1.905828 -0.877803 -0.041735
C4 -0.742501 1.136670 -0.277402
C5 2.436732 -0.476052 -0.147872
N6 -1.977996 0.429786 -0.101702
N7 -0.784390 -1.688519 -0.173779
N8 1.573266 -1.544610 -0.274320
N9 -3.050347 -1.584309 0.154279
H10 -3.932183 -1.108486 0.036072
H11 -3.026068 -2.571647 -0.051224
O12 3.669993 -0.540748 -0.247146
N13 1.756123 0.718204 0.059886
O14 0.162691 0.517753 1.809989
H15 2.235759 1.475878 0.529564
O16 -0.386465 1.250501 -1.631703
H17 -1.205574 1.393936 -2.124340
H18 -1.316890 2.412910 1.067471
O19 -0.873201 2.453830 0.210739
H20 0.745112 -0.089305 2.285176

Cartesian coordinates for the structures in Fig. 7, optimized at SMD-ωB97XD/aug-cc-pVQZ//SMD-ωB97XD/6-31+G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

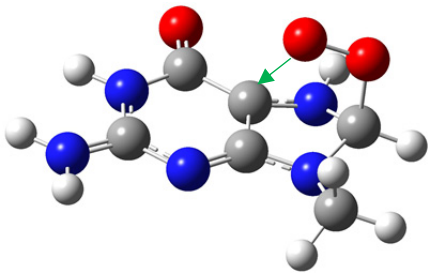
TS1^{+}(9MG) (open-shell)



C1 -0.088637 0.854624 -0.396276
C2 0.069589 -0.550147 -0.347981
C3 -2.079036 -0.897511 0.138455
C4 -1.377909 1.438223 -0.166377
C5 2.048181 0.389011 -0.695391
N6 -2.323493 0.451466 0.101392
N7 -0.872658 -1.438374 -0.088305
O8 -1.666075 2.630113 -0.189921
N9 1.368854 -0.807754 -0.658112
N10 -3.096429 -1.696059 0.416653
H11 -4.028346 -1.337858 0.576775
H12 -2.938831 -2.694323 0.441036
N13 1.107507 1.388487 -0.728209
H14 -3.268478 0.782709 0.280468
H15 2.997157 0.490816 -1.203160
O16 1.779435 0.284174 1.832655
O17 2.707501 0.541926 1.019924
H18 1.333895 2.375954 -0.784816
C19 2.014982 -2.111886 -0.572455
H20 2.061512 -2.435719 0.468962
H21 1.446174 -2.828328 -1.164048
H22 3.020539 -2.021210 -0.980260

[8-OO9MG + H]$^{+}$ (open-shell)
O1 2.215168 0.295474 1.712412
O2 2.905044 0.485670 0.625413
C3 -0.129793 0.861903 -0.325489
C4 0.015176 -0.558348 -0.292116
C5 -2.157084 -0.867381 0.150568
C6 -1.416603 1.454035 -0.119446
C7 2.059295 0.368856 -0.600843
N8 -2.386901 0.480115 0.115236
N9 -0.947918 -1.423603 -0.054274
O10 -1.686313 2.651722 -0.135501
N11 1.299210 -0.839372 -0.580965
N12 -3.181922 -1.661244 0.401316
H13 -4.114373 -1.298362 0.549770
H14 -3.030647 -2.660905 0.420405
N15 1.066354 1.396271 -0.615262
H16 -3.331010 0.823331 0.274226
H17 2.800322 0.437356 -1.395475
H18 1.293439 2.383811 -0.646339
C19 1.919071 -2.155104 -0.509172
H20 2.002341 -2.483654 0.529249
H21 1.316335 -2.863530 -1.077127
H22 2.910279 -2.089917 -0.956665

TS2^{+}(9MG) (open-shell)



C1 -1.304826 1.426025 -0.172833
C2 0.006470 0.840007 -0.395707
H3 -3.203672 0.768049 0.225893
C4 -2.011915 -0.910854 0.063363
C5 2.149150 0.388032 -0.442097
N6 -2.253646 0.441301 0.062071
N7 1.154986 1.367037 -0.800521
N8 1.459522 -0.853078 -0.603784
N9 -0.796835 -1.462972 -0.133763
C10 0.163456 -0.598877 -0.353703
N11 -3.032099 -1.709924 0.281897
H12 -2.874828 -2.709800 0.283721
H13 -3.969711 -1.356579 0.426742
O14 -1.572012 2.614751 -0.188598
H15 3.113290 0.482127 -0.928023
H16 1.363959 2.362202 -0.761513
O17 1.252444 0.359126 1.671935
O18 2.359659 0.677555 0.991864
C19 2.113631 -2.128804 -0.339074
H20 1.556179 -2.921013 -0.837277
H21 3.121906 -2.087010 -0.748443
H22 2.152861 -2.319169 0.736309

endoperoxide
[5,8-OO-9MG + H]$^{+}$
C1 1.196079 -1.380888 -0.187305

C2 -0.192875 -0.795442 -0.096602
H3 3.138711 -0.782356 -0.055043
C4 1.979905 0.929577 0.053202
C5 -2.175848 -0.317525 -0.315996
N6 2.182448 -0.431754 -0.049306
N7 -1.231447 -1.170598 -1.006289
N8 -1.511006 0.983385 -0.379037
N9 0.775754 1.530024 -0.025619
C10 -0.230069 0.710590 -0.196148
N11 3.041486 1.677820 0.224729
H12 2.925926 2.681915 0.285978
O13 1.421420 -2.560607 -0.337225
H14 -3.208532 -0.322889 -0.649258
C15 -2.179783 2.259755 -0.177658
H16 -2.363597 2.424583 0.886669
H17 -1.543803 3.052260 -0.570277
H18 -3.122354 2.246174 -0.723048
O19 -2.135502 -0.758380 1.050533
O20 -0.723844 -1.054830 1.235472
H21 3.973095 1.285263 0.288376
H22 -1.481140 -2.152944 -0.881945

[8-H-8-OOH9MG + H]$^+$
C1 -1.456022 1.486755 -0.132105
C2 -0.125206 0.853930 -0.311658
H3 -3.378998 0.905125 0.229165
C4 -2.236579 -0.820675 0.178842
C5 1.963689 0.329064 -0.661098
N6 -2.436193 0.543075 0.100713
N7 0.998402 1.415677 -0.523836
N8 1.216501 -0.914005 -0.447022
N9 -1.048837 -1.431596 0.010031
C10 -0.045349 -0.616999 -0.231543
N11 -3.290092 -1.558985 0.437287
H12 -3.181379 -2.563638 0.495557
H13 -4.208851 -1.155138 0.572066
O14 -1.681594 2.677293 -0.181494
H15 2.389946 0.350306 -1.668295
O16 2.618225 0.423093 1.533813
O17 3.066044 0.451121 0.178506
H18 2.750696 1.345568 1.807816
C19 1.828843 -2.232930 -0.420175
H20 1.887884 -2.594888 0.608182
H21 1.234398 -2.919641 -1.023975
H22 2.830183 -2.153784 -0.840900

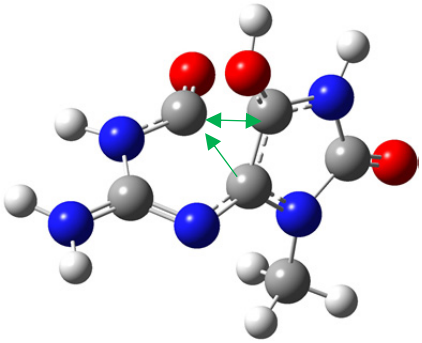
[8-OOH9MG + H]$^+$
C1 -1.323813 1.575530 -0.003546
C2 -0.160918 0.765159 -0.004664
H3 -3.353784 1.281877 0.001127
C4 -2.494512 -0.593495 0.000294
C5 1.853975 -0.071431 0.000430
N6 -2.470708 0.778639 -0.000825
N7 1.196582 1.075082 -0.004865
N8 1.016572 -1.120412 0.005525
N9 -1.393125 -1.334297 -0.002662
C10 -0.273146 -0.605788 -0.002979
N11 -3.692558 -1.183431 0.001524
H12 -3.738441 -2.191230 0.018046
H13 -4.549526 -0.649795 0.022249
O14 -1.401050 2.808044 -0.004332
H15 4.232347 1.067572 -0.767583
H16 1.626581 1.993845 0.006074
O17 3.165259 -0.260964 0.004927
O18 3.812973 0.996445 0.108868
C19 1.411410 -2.528227 -0.009480
H20 1.859355 -2.775591 -0.971824
H21 2.118210 -2.713766 0.798812
H22 0.512496 -3.120669 0.146186

[9MOG^{ox} + H]$^+$
C1 1.302950 1.457338 0.000001
C2 -0.087029 0.930741 -0.000001
H3 3.213372 0.714656 0.000004
C4 1.943821 -0.907447 0.000003
C5 -2.207728 0.533725 -0.000005
N6 2.234020 0.432456 0.000004
N7 -1.189029 1.570996 -0.000004
N8 -1.591891 -0.732344 0.000000
N9 0.677157 -1.424243 0.000003
C10 -0.267575 -0.541817 0.000001
N11 2.935444 -1.752654 0.000004
H12 2.732860 -2.746285 0.000004
H13 3.902956 -1.446040 0.000004
O14 1.605095 2.627741 0.000000
O15 -3.386600 0.746637 -0.000009
C16 -2.292443 -2.010576 0.000001
H17 -2.023793 -2.571564 -0.895563
H18 -2.023785 -2.571566 0.895561
H19 -3.361453 -1.805474 0.000006

[5-OH9MOG + H]$^+$
C1 1.185287 -1.330161 -0.399144
C2 -0.055552 -0.845050 0.347865
H3 3.109724 -0.676741 -0.719489
C4 1.990743 0.937476 -0.071207
C5 -2.234022 -0.330604 -0.143022
N6 2.183575 -0.375688 -0.421553
N7 -1.315172 -1.341490 -0.105146
N8 -1.516661 0.897473 -0.023577
N9 0.759688 1.491783 0.063907
C10 -0.220748 0.642791 0.117540

N11 3.039786 1.706281 0.053670
H12 2.908629 2.689382 0.261199
H13 3.980843 1.344164 -0.051229
O14 1.332090 -2.452746 -0.826138
H15 -1.612623 -2.288383 0.101223
H16 0.361956 -1.952892 1.900527
O17 0.185698 -1.016412 1.723059
O18 -3.432713 -0.408078 -0.294909
C19 -2.113599 2.206642 -0.248535
H20 -1.780072 2.608281 -1.206711
H21 -3.194831 2.081934 -0.254572
H22 -1.825389 2.877070 0.560858

TS3a^{+}(9MG)

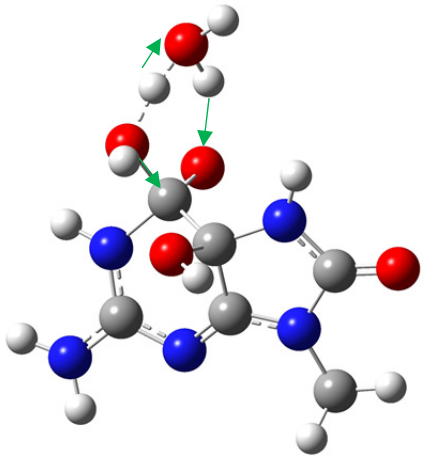


C1 0.327468 -1.035223 -0.693437
C2 -0.007211 0.342285 -0.574266
C3 -2.164500 0.475193 -0.104790
C4 -0.532052 -0.729229 1.045673
C5 2.195640 0.098661 -0.144844
N6 -1.831799 -0.375735 0.949019
N7 -1.199302 0.910144 -0.874522
O8 0.084149 -1.200605 1.955707
N9 1.153314 1.012423 -0.291338
N10 -3.432488 0.821277 -0.242223
H11 -4.144805 0.464434 0.379302
H12 -3.693425 1.458959 -0.981733
O13 3.328973 0.342712 0.220924
N14 1.671840 -1.140879 -0.479142
O15 -0.432020 -1.928363 -1.299454
H16 2.175348 -2.009234 -0.331503
H17 -2.469726 -0.539300 1.725279
H18 -0.180695 -2.838919 -1.074360
C19 1.218214 2.361948 0.253945
H20 1.052843 2.337451 1.333402
H21 2.201039 2.775347 0.034651
H22 0.454293 2.968894 -0.228695

[9MSp + H]$^{+}$
C1 -0.730333 1.393140 -0.192346
C2 0.066316 0.106697 -0.169807
C3 2.218341 -0.148888 -0.470057
C4 0.754477 -0.063379 1.228487
C5 -2.220665 -0.300912 -0.287986
N6 2.061698 -0.220121 0.915866
N7 1.115368 0.053938 -1.141204
O8 0.215328 -0.071169 2.314642
N9 -1.000696 -0.866380 -0.344967
N10 3.432068 -0.283896 -0.988550
H11 4.234221 -0.455554 -0.399741
H12 3.550903 -0.261219 -1.990964
O13 -3.323095 -0.804433 -0.287612
N14 -2.004170 1.125008 -0.244527
O15 -0.144693 2.524932 -0.152651
H16 -2.764322 1.803122 -0.262219
H17 2.802691 -0.394790 1.586247
H18 -0.747519 3.291229 -0.160028
C19 -0.776039 -2.298787 -0.206663
H20 -0.756797 -2.589760 0.846898
H21 -1.576772 -2.828827 -0.721243
H22 0.174811 -2.545910 -0.680070

[5-OH9MOG·2H$_2$O + H]$^{+}$
C1 -0.123439 -0.222368 0.181072
C2 1.068115 0.720242 0.195630
C3 2.517687 -0.965483 -0.068131
C4 0.215556 -1.428209 -0.693866
C5 -0.786680 1.939905 -0.174674
N6 1.549392 -1.772905 -0.615321
N7 2.310264 0.337467 0.237270
O8 -0.599418 -2.063863 -1.320944
N9 0.608189 1.963581 0.154252
N10 3.718470 -1.459611 0.082267
H11 3.934054 -2.422479 -0.149328
H12 4.458775 -0.858232 0.423476
O13 -1.450460 2.938615 -0.357554
N14 -1.161221 0.638152 -0.273743
O15 -0.338927 -0.796119 1.449279
H16 -0.471893 -0.095918 2.107963
H17 -2.147167 0.349640 -0.356139
H18 1.825219 -2.654387 -1.043880
O19 -2.956533 -2.162282 1.285447
H20 -2.059724 -1.823494 1.425098
H21 -4.529968 0.371104 -0.311329
O22 -3.832041 -0.234060 -0.588858
H23 -4.040124 -0.472251 -1.500051
H24 -3.328503 -1.563858 0.613249
C25 1.409456 3.178161 0.145290
H26 1.883918 3.304059 -0.829766
H27 0.748599 4.018531 0.350548
H28 2.166013 3.108682 0.926202

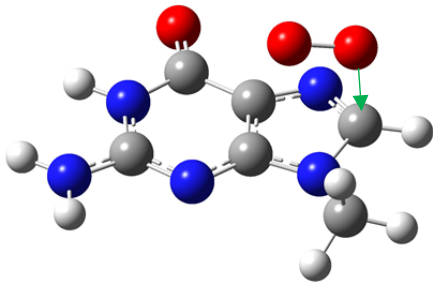
TS3b^{+}(9MG) PCM-B3LYP/6-31+G(d,p)



C1 0.009519 -0.359092 0.618948
C2 -1.056543 0.596407 0.074039
C3 0.431821 2.284708 -0.128885
C4 1.308582 -0.053608 -0.205548
C5 -1.940685 -1.497082 0.041062
N6 1.466718 1.439479 -0.103232
N7 -0.874175 1.858181 -0.165124
O8 1.392298 -0.542105 -1.382401
N9 -2.186779 -0.096225 -0.128740
N10 0.614043 3.601127 -0.169393
H11 1.528882 4.029728 -0.171274
H12 -0.200304 4.198565 -0.204829
O13 -2.767232 -2.368064 -0.137175
N14 -0.626899 -1.621574 0.404947
O15 0.324146 -0.095575 1.974873
H16 -0.411817 -0.353607 2.552018
H17 -0.227105 -2.515461 0.657273
H18 2.411657 1.788620 -0.219333
O19 2.507260 -0.531942 0.667400
H20 2.237294 -0.608504 1.603611
H21 2.442392 -1.852226 -1.378881
O22 3.167867 -2.267277 -0.810567
H23 2.956174 -3.198760 -0.637080
H24 2.940629 -1.524713 0.105131
C25 -3.445791 0.444926 -0.634105
H26 -3.292843 0.879119 -1.624526
H27 -4.156904 -0.377425 -0.692610
H28 -3.814530 1.209893 0.051177

[*gem*-9Mdiol + H]$^{+}$
C1 -0.068291 -0.713173 0.452226
C2 -0.397690 0.737400 0.114005
C3 1.779097 1.275474 0.009147
C4 1.174864 -1.089126 -0.381166
C5 -2.309066 -0.451257 -0.019840
N6 2.137673 -0.003549 -0.158170
N7 0.470697 1.688363 -0.012293
N8 -1.722009 0.842272 -0.022867
N9 2.698547 2.205407 0.164818
H10 3.684789 1.978714 0.158630
H11 2.412292 3.167730 0.284266
O12 -3.498091 -0.663740 -0.147353
N13 -1.300154 -1.357338 0.115037
O14 0.318072 -0.875224 1.787709
H15 -1.497310 -2.312674 0.387377
O16 0.782008 -1.176663 -1.701559
H17 1.562128 -1.304502 -2.259950
H18 1.871324 -2.294301 0.967139
O19 1.755108 -2.286736 0.004951
H20 -0.404627 -0.620815 2.379023
C21 -2.456974 2.065012 -0.305931
H22 -2.249857 2.404358 -1.322316
H23 -3.519016 1.852677 -0.196063
H24 -2.162622 2.830191 0.412090
H25 3.121201 -0.254533 -0.176514

TS1(9MG) (open-shell)

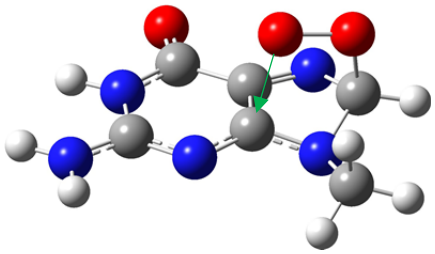


C1 0.032083 0.872266 -0.436413
C2 0.210123 -0.544415 -0.356655
C3 -1.937193 -0.957048 0.063092
C4 -1.300976 1.404796 -0.229445
C5 2.090588 0.508742 -0.656792
N6 -2.217524 0.392359 0.026130
N7 -0.725232 -1.469402 -0.132564
O8 -1.644787 2.580972 -0.265254
N9 1.508335 -0.750533 -0.659967
N10 -2.958283 -1.769437 0.312877
H11 -3.898807 -1.422297 0.437699
H12 -2.791231 -2.765352 0.337371
N13 1.163365 1.496915 -0.736905
H14 -3.175039 0.693067 0.188150
H15 3.118503 0.633908 -0.963124
O16 1.135117 0.314434 1.747346
O17 2.268672 0.688153 1.259029

C18 2.239658 -1.988487 -0.448595
H19 2.328924 -2.193000 0.621277
H20 1.714855 -2.807586 -0.939615
H21 3.230462 -1.881645 -0.888865

8-OO9MG
C1 -1.450682 1.480298 -0.105006
C2 -0.109610 0.871849 -0.278785
H3 -3.368030 0.866198 0.232606
C4 -2.201441 -0.843688 0.156671
C5 2.006837 0.390281 -0.612394
N6 -2.419700 0.519845 0.103899
N7 1.009074 1.456072 -0.451017
N8 1.251419 -0.874673 -0.447927
N9 -1.009608 -1.433944 -0.016483
C10 -0.009568 -0.597927 -0.234729
N11 -3.252852 -1.597693 0.393129
H12 -3.135321 -2.601971 0.429172
H13 -4.176152 -1.204949 0.525440
O14 -1.698293 2.668670 -0.138105
H15 2.387970 0.445345 -1.637967
O16 2.660228 0.439575 1.602473
O17 3.089472 0.491335 0.212332
C18 1.881606 -2.180882 -0.401300
H19 1.940539 -2.527991 0.632851
H20 1.303413 -2.887382 -0.998241
H21 2.885151 -2.092722 -0.815417

TS2(9MG)



C1 -1.395695 1.385846 -0.179603
C2 0.006755 0.952357 -0.345583
C3 -1.857133 -1.022523 0.029683
C4 2.103484 0.665684 -0.336370
N5 -2.235727 0.313049 0.028309
N6 1.060048 1.654390 -0.556619
N7 1.556318 -0.607562 -0.750015
N8 -0.613304 -1.458307 -0.137104
C9 0.298657 -0.487948 -0.249950
N10 -2.836521 -1.895774 0.199862
H11 -2.615032 -2.881828 0.205231
H12 -3.801330 -1.607193 0.292767
O13 -1.798965 2.534761 -0.214076
H14 3.082407 0.909496 -0.732279
O15 1.004905 0.031056 1.568665
O16 2.214075 0.590227 1.113709
H17 -3.220526 0.534122 0.153001
C18 2.348239 -1.810764 -0.532083
H19 1.857579 -2.655067 -1.015676
H20 3.325673 -1.664153 -0.991704
H21 2.469558 -2.020205 0.534684

endoperoxide
4,8-OO-9MG
C1 -1.450621 1.372863 -0.146483
C2 -0.021560 1.003510 -0.242667
C3 -1.794619 -1.063377 0.006591
C4 2.080411 0.762232 -0.254745
N5 -2.241967 0.266714 0.006010
N6 1.000738 1.754002 -0.406261
N7 1.577940 -0.454183 -0.841210
N8 -0.547238 -1.442997 -0.065643
C9 0.388234 -0.418340 -0.027893
N10 -2.778996 -1.962504 0.088417
H11 -2.542131 -2.943254 0.108014
H12 -3.752147 -1.694265 0.074487
O13 -1.892986 2.509844 -0.197009
H14 3.064659 1.096082 -0.564116
O15 2.130510 0.492070 1.171158
O16 0.950725 -0.306138 1.376104
H17 -3.240132 0.438216 0.087546
C18 2.444529 -1.625963 -0.671972
H19 1.984814 -2.481810 -1.165635
H20 3.395726 -1.420743 -1.165009
H21 2.631643 -1.873215 0.376496

8-H-8-OOH9MG
C1 -1.532661 1.438400 -0.128479
C2 -0.169773 0.858001 -0.318492
C3 -2.239144 -0.769677 0.178684
C4 1.941119 0.377420 -0.650750
N5 -2.514236 0.550101 0.119604
N6 0.948391 1.440836 -0.517093
N7 1.218232 -0.880239 -0.517782
N8 -1.041438 -1.427059 -0.022311
C9 -0.055402 -0.611445 -0.267178
N10 -3.256574 -1.569678 0.468414
H11 -3.116512 -2.568225 0.523850
H12 -4.173026 -1.179875 0.635008
O13 -1.712720 2.661431 -0.202793
H14 2.437592 0.450309 -1.621877
O15 2.474254 0.350964 1.587958
O16 2.993263 0.497999 0.267147

H17 2.437801 1.268822 1.902106
C18 1.859769 -2.181563 -0.473984
H19 1.955384 -2.526463 0.558549
H20 1.267682 -2.896492 -1.047183
H21 2.848640 -2.095769 -0.923581

8-OOH9MG

C1 -1.491802 1.502970 -0.015551
C2 -0.224219 0.865433 -0.105411
C3 -2.374318 -0.796945 0.099522
C4 1.808994 0.351890 -0.268097
N5 -2.525697 0.568645 0.086033
N6 1.040667 1.403190 -0.222096
N7 1.145399 -0.849558 -0.183209
N8 -1.199269 -1.394798 0.030153
C9 -0.174440 -0.523245 -0.074345
N10 -3.503012 -1.529537 0.152351
H11 -3.408886 -2.520030 0.322988
H12 -4.382320 -1.092798 0.388602
O13 -1.748037 2.715827 -0.019603
H14 3.928697 1.109129 1.140014
O15 3.151264 0.396674 -0.439496
O16 3.783475 0.193007 0.848774
H17 -3.461719 0.957335 0.151233
C18 1.713405 -2.188069 -0.215897
H19 1.216325 -2.774915 -0.989096
H20 2.773851 -2.107866 -0.448737
H21 1.588098 -2.672712 0.753635

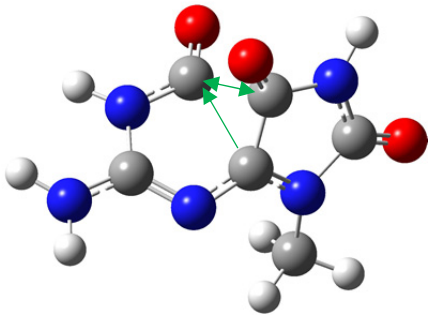
9MOG^{ox}

C1 1.366246 1.418465 -0.005306
C2 -0.042711 0.918912 -0.008393
C3 1.989472 -0.828454 0.004111
C4 -2.170404 0.527968 0.004456
N5 2.325627 0.466716 0.004816
N6 -1.149277 1.557580 0.005670
N7 -1.571514 -0.732983 -0.038393
N8 0.712490 -1.415132 -0.017134
C9 -0.232510 -0.548002 -0.023577
N10 2.962706 -1.718533 0.026361
H11 2.747519 -2.706397 0.026404
H12 3.927114 -1.414151 0.044691
O13 1.595988 2.629737 -0.009841
O14 -3.353627 0.751804 0.038051
C15 -2.276930 -2.004508 -0.000842
H16 -1.908407 -2.647631 -0.800422
H17 -2.127567 -2.486354 0.966745
H18 -3.336760 -1.807623 -0.155024

5-OH9MOG

C1 1.255012 -1.302843 -0.396633
C2 -0.010686 -0.839311 0.335534
C3 2.031697 0.859953 -0.112548
C4 -2.195484 -0.323543 -0.141278
N5 2.274934 -0.417638 -0.434032
N6 -1.269046 -1.332236 -0.129154
N7 -1.500670 0.898640 -0.005062
N8 0.788095 1.483382 -0.017885
C9 -0.184084 0.647506 0.096857
N10 3.061868 1.672130 0.050181
H11 2.910993 2.651119 0.249362
H12 4.003889 1.313695 -0.021317
O13 1.328918 -2.455591 -0.827954
H14 -1.564982 -2.275783 0.091598
H15 0.960909 -0.861773 2.064225
O16 0.095433 -1.123342 1.718290
O17 -3.399192 -0.422986 -0.289009
C18 -2.101062 2.205218 -0.220706
H19 -1.773455 2.618942 -1.176546
H20 -3.182861 2.082530 -0.224275
H21 -1.814379 2.874796 0.590653

TS3a(9MG)



C1 0.314611 -0.933354 -0.766869
C2 0.017858 0.413703 -0.596955
C3 -2.136503 0.525342 -0.028985
C4 -0.786783 -0.963734 1.085511
C5 2.195684 0.103888 -0.076621
N6 -1.939785 -0.419420 0.962424
N7 -1.173382 1.026169 -0.775784
O8 -0.142090 -1.677245 1.797677
N9 1.184650 1.040164 -0.196357
N10 -3.392941 0.955056 -0.162248
H11 -4.113262 0.614828 0.455896
H12 -3.604045 1.687766 -0.823370
O13 3.329871 0.303780 0.361995
N14 1.672990 -1.083862 -0.522284
O15 -0.394032 -1.808182 -1.509900
H16 2.145988 -1.970084 -0.397721
H17 -0.311749 -2.704890 -1.152519

C18 1.264356 2.368950 0.385663
H19 1.071216 2.329644 1.460709
H20 2.259844 2.773145 0.205670
H21 0.525964 3.007251 -0.097548

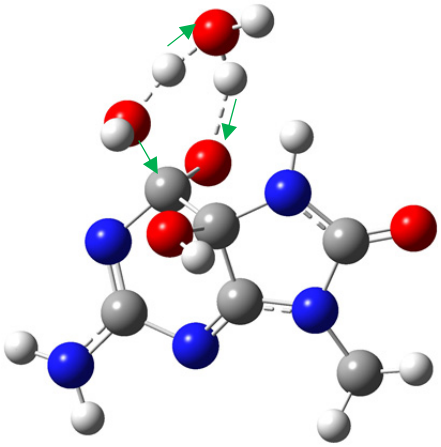
9MSp

C1 -0.657809 1.391207 -0.199413
C2 0.109799 0.104304 -0.218326
C3 2.247634 -0.168346 -0.338511
C4 0.759930 -0.122915 1.210728
C5 -2.182834 -0.265777 -0.297976
N6 2.062771 -0.290615 1.027382
N7 1.203577 0.053153 -1.125112
O8 0.084421 -0.147059 2.249136
N9 -0.978980 -0.845011 -0.442452
N10 3.492330 -0.273267 -0.819068
H11 4.256077 -0.484501 -0.196546
H12 3.659148 -0.241181 -1.812947
O13 -3.296549 -0.754660 -0.255103
N14 -1.942614 1.149584 -0.214070
O15 -0.064577 2.524163 -0.143080
H16 -2.689867 1.839179 -0.168412
H17 -0.668609 3.286694 -0.094824
C18 -0.779904 -2.277105 -0.282908
H19 -0.768099 -2.553239 0.775486
H20 -1.585083 -2.806120 -0.791864
H21 0.169585 -2.545505 -0.746850

5-OH9MOG·2H2O

C1 0.160723 0.085297 0.207981
C2 -1.278398 -0.382150 0.117614
C3 -1.932749 1.745226 -0.062772
C4 0.281525 1.381788 -0.605973
C5 0.040970 -2.176282 -0.208739
N6 -0.773965 2.211795 -0.549627
N7 -2.292650 0.409293 0.092851
O8 1.331729 1.649811 -1.200642
N9 -1.276693 -1.723266 0.041407
N10 -2.894271 2.609538 0.205308
H11 -2.734460 3.599867 0.081196
H12 -3.797919 2.281840 0.517669
O13 0.347394 -3.341743 -0.377215
N14 0.850895 -1.077810 -0.263616
O15 0.502906 0.458298 1.525930
H16 0.264995 -0.251928 2.141501
H17 1.855702 -1.173307 -0.173012
H18 3.653240 0.400431 0.775355
O19 3.437296 0.431787 1.727654
H20 2.470085 0.496662 1.744608
H21 2.935111 0.805626 -1.186041
O22 3.832735 0.437844 -1.061568
H23 3.784837 -0.466029 -1.393112
C24 -2.456615 -2.564218 -0.080564
H25 -2.902921 -2.447311 -1.070477
H26 -2.156046 -3.599491 0.071992
H27 -3.175055 -2.279142 0.687517

TS3b(9MG)

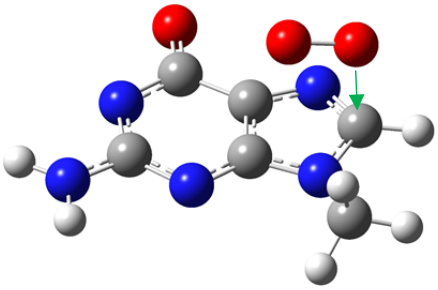


C1 0.060446 -0.256356 0.660463
C2 -0.833767 0.837455 0.107200
C3 0.999327 2.103531 -0.194009
C4 1.318670 -0.213952 -0.253591
C5 -2.047491 -1.058297 0.134683
N6 1.853103 1.129330 -0.252856
N7 -0.414010 1.999407 -0.229850
O8 1.128640 -0.751578 -1.443269
N9 -2.088486 0.340333 -0.017546
N10 1.417572 3.390300 -0.134197
H11 2.394554 3.585860 -0.295869
H12 0.751769 4.119598 -0.340115
O13 -2.985388 -1.808321 -0.092882
N14 -0.804066 -1.394956 0.571176
O15 0.481130 0.010896 1.978597
H16 -0.284410 0.010388 2.568853
H17 -0.479298 -2.351970 0.550152
H18 2.229226 -2.174605 0.041526
O19 2.369856 -1.051056 0.477095
H20 2.249987 -0.981538 1.438985
H21 1.430588 -2.307090 -1.289656
O22 1.935886 -3.020572 -0.759634
H23 1.290994 -3.641334 -0.392715
C24 -3.211354 1.050376 -0.603357
H25 -3.054557 1.200135 -1.674339
H26 -4.113383 0.462097 -0.442229
H27 -3.320240 2.016062 -0.109266

***gem*-9Mdiol**

C1 -0.033625 -0.705369 0.466121
C2 -0.364872 0.742974 0.143876
C3 1.836811 1.178640 0.006687
C4 1.207075 -1.042137 -0.385625
C5 -2.281246 -0.436163 -0.001595
N6 2.227341 -0.050834 -0.185752
N7 0.510342 1.665094 -0.018297
N8 -1.708449 0.850359 0.028336
N9 2.739191 2.153360 0.213185
H10 3.725045 1.943954 0.182487
H11 2.437732 3.113543 0.266453
O12 -3.472952 -0.660140 -0.147808
N13 -1.275328 -1.345052 0.131458
O14 0.340350 -0.888185 1.807986
H15 -1.474996 -2.304041 0.384791
O16 0.765796 -1.095039 -1.715000
H17 1.542055 -0.975715 -2.278565
H18 2.197644 -2.261283 0.757832
O19 1.704702 -2.317828 -0.071047
H20 -0.379079 -0.603832 2.388281
C21 -2.426196 2.060441 -0.333796
H22 -2.222836 2.326842 -1.373570
H23 -3.491560 1.877441 -0.202212
H24 -2.116541 2.871823 0.324948

TS1^{-}(9MG) (open-shell)

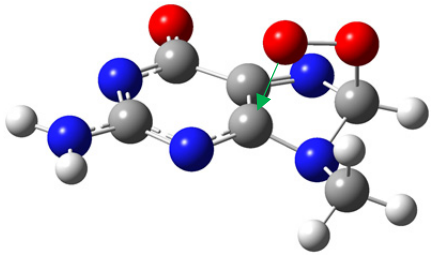


C1 -0.012025 0.858156 -0.438807
C2 0.171463 -0.555115 -0.364376
C3 -1.979028 -0.880704 0.073384
C4 -1.363542 1.365515 -0.221951
C5 2.048589 0.498358 -0.714088
N6 -2.307805 0.429164 0.042906
N7 -0.766108 -1.460083 -0.130682
O8 -1.634286 2.588279 -0.279712
N9 1.479097 -0.759048 -0.672405
N10 -2.983919 -1.732920 0.343847
H11 -3.920397 -1.382832 0.469975
H12 -2.813704 -2.726583 0.345872
N13 1.123806 1.481563 -0.758580
H14 3.077839 0.625888 -1.015621
O15 1.126872 0.335800 1.774253
O16 2.273224 0.686583 1.305106
C17 2.217125 -1.989677 -0.457838
H18 2.293194 -2.204466 0.611562
H19 1.710625 -2.813242 -0.961719
H20 3.214980 -1.874000 -0.880803

[8-OO9MG – H]$^{-}$

C1 -1.516584 1.443926 -0.094996
C2 -0.152981 0.865988 -0.276995
C3 -2.232087 -0.768373 0.164264
C4 1.971672 0.393111 -0.614610
N5 -2.504363 0.554947 0.123795
N6 0.966138 1.451783 -0.458170
N7 1.230053 -0.872411 -0.468930
N8 -1.036179 -1.422512 -0.013874
C9 -0.039678 -0.602361 -0.236585
N10 -3.266174 -1.567613 0.406866
H11 -3.136589 -2.568215 0.439480
H12 -4.184819 -1.173890 0.547160
O13 -1.697934 2.669838 -0.149933
H14 2.381421 0.461810 -1.627907
O15 3.049704 0.501764 0.230054
O16 2.615771 0.429459 1.617264
C17 1.866151 -2.172672 -0.415100
H18 1.933406 -2.521172 0.618958
H19 1.292360 -2.888174 -1.006799
H20 2.868611 -2.085916 -0.833643

TS2^{-}(9MG)



C1 -1.485315 1.331128 -0.156970
C2 -0.049811 0.966826 -0.302503
C3 -1.869114 -0.977258 0.017270
C4 2.061170 0.721182 -0.289679
N5 -2.330886 0.308578 0.036296
N6 0.992776 1.699206 -0.468771
N7 1.549994 -0.532307 -0.799480
N8 -0.614778 -1.443174 -0.163196
C9 0.296355 -0.464614 -0.206418
N10 -2.819019 -1.906000 0.186049

H11 -2.577665 -2.885047 0.181755
H12 -3.784502 -1.628846 0.271457
O13 -1.849844 2.522576 -0.213791
H14 3.039134 1.020120 -0.650913
O15 0.955466 -0.123551 1.504815
O16 2.158937 0.537881 1.150010
C17 2.377352 -1.715952 -0.593757
H18 1.911113 -2.570186 -1.084900
H19 3.349173 -1.541804 -1.057548
H20 2.515844 -1.941481 0.467932

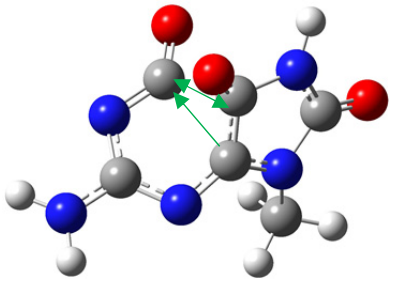
endoperoxide
[4,8-OO-9MG – H]$^-$
C1 -1.510809 1.323977 -0.137634
C2 -0.063284 0.991911 -0.237190
C3 -1.836162 -1.000309 0.008767
C4 2.047513 0.767659 -0.261252
N5 -2.335666 0.285966 0.007631
N6 0.960321 1.745959 -0.405071
N7 1.551336 -0.455698 -0.843824
N8 -0.582543 -1.437266 -0.067004
C9 0.352991 -0.426790 -0.038866
N10 -2.801922 -1.935133 0.101082
H11 -2.562049 -2.913850 0.097331
H12 -3.769424 -1.655580 0.091769
O13 -1.892721 2.514608 -0.194902
H14 3.027593 1.107014 -0.579582
O15 2.120535 0.490816 1.165322
O16 0.941110 -0.304781 1.383397
C17 2.420805 -1.622780 -0.673090
H18 1.962108 -2.482893 -1.161363
H19 3.371933 -1.420724 -1.168509
H20 2.611442 -1.867914 0.375702

[8-OOH9MG – H]$^-$
C1 -1.554614 1.472626 -0.013309
C2 -0.264787 0.857423 -0.097283
C3 -2.408056 -0.716111 0.098624
C4 1.777183 0.344767 -0.265996
N5 -2.611095 0.614369 0.083307
N6 1.005590 1.395341 -0.213493
N7 1.117859 -0.857178 -0.183186
N8 -1.242805 -1.379850 0.033370
C9 -0.208656 -0.529447 -0.070676
N10 -3.545023 -1.490471 0.142295
H11 -3.416331 -2.440775 0.459702
H12 -4.368334 -1.029582 0.502650
O13 -1.736000 2.727692 -0.030405
H14 3.888712 1.113818 1.146927
O15 3.121140 0.393502 -0.437388
O16 3.760686 0.196445 0.852822
C17 1.685520 -2.192774 -0.231737
H18 1.196755 -2.770873 -1.017671
H19 2.748655 -2.112482 -0.453718
H20 1.552724 -2.695597 0.728097

[9MOG^{ox} – H]$^-$
C1 1.447624 1.333259 -0.003996
C2 0.028077 0.884383 -0.012037
C3 2.021600 -0.975852 0.005045
C4 -2.115823 0.575047 0.000945
N5 2.361120 0.369197 0.008180
N6 -1.062128 1.560686 0.004643
N7 -1.573378 -0.697024 -0.057853
N8 0.685282 -1.476760 -0.030244
C9 -0.210808 -0.567568 -0.036029
N10 2.924721 -1.892452 0.036043
O11 1.706142 2.560876 -0.004900
O12 -3.297832 0.846931 0.044754
C13 -2.321911 -1.938730 0.014549
H14 -1.975969 -2.621729 -0.762123
H15 -2.194282 -2.400782 0.995726
H16 -3.374830 -1.713366 -0.149870
H17 3.836721 -1.435332 0.061188

[5-OH9MOG – H]$^-$
C1 1.244930 -1.313892 -0.352922
C2 0.001286 -0.854382 0.407806
C3 2.030232 0.845029 -0.097864
C4 -2.192511 -0.336743 -0.128016
N5 2.276832 -0.431008 -0.407069
N6 -1.282703 -1.347470 -0.119159
N7 -1.494699 0.884703 0.009668
N8 0.790179 1.470443 -0.004539
C9 -0.178711 0.624380 0.118211
N10 3.064312 1.666069 0.048893
H11 2.910720 2.646081 0.236244
H12 4.006205 1.310718 -0.026828
O13 1.345455 -2.475580 -0.773502
H14 -1.606022 -2.264617 0.165405
O15 0.189728 -1.089213 1.735898
O16 -3.407004 -0.415274 -0.267313
C17 -2.087039 2.187948 -0.238639
H18 -1.847613 2.533321 -1.247131
H19 -3.166662 2.099668 -0.127516
H20 -1.708633 2.902176 0.493141

TS3a^{-}(9MG)



C1 0.227571 -0.958919 -0.778596
C2 0.002686 0.445368 -0.589371
C3 -2.134550 0.486613 -0.003366
C4 -0.675098 -0.981575 0.912019
C5 2.174527 0.068033 -0.115110
N6 -1.901650 -0.493429 0.925753
N7 -1.177718 1.072219 -0.714002
O8 -0.113240 -1.748546 1.682865
N9 1.183847 1.043837 -0.222134
N10 -3.402542 0.902050 -0.131543
H11 -4.108632 0.543149 0.491989
H12 -3.612727 1.698628 -0.713572
O13 3.314660 0.258387 0.312395
N14 1.626792 -1.098026 -0.546660
O15 -0.431561 -1.815400 -1.473881
H16 2.085712 -1.989007 -0.413359
C17 1.281139 2.320070 0.470686
H18 1.089907 2.194278 1.539890
H19 2.279819 2.728563 0.320937
H20 0.548297 3.004761 0.045623

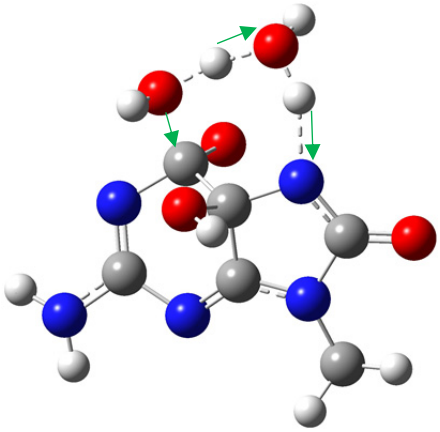
[9MSp – H]$^{-}$

C1 -0.620417 1.470337 -0.173450
C2 0.107909 0.126255 -0.205701
C3 2.246850 -0.149230 -0.349070
C4 0.759041 -0.128345 1.193836
C5 -2.188794 -0.185335 -0.303609
N6 2.068466 -0.281006 1.019016
N7 1.202185 0.064195 -1.125545
O8 0.097693 -0.173888 2.248843
N9 -0.992173 -0.797392 -0.458204
N10 3.504205 -0.216351 -0.831246
H11 4.234029 -0.561742 -0.227475
H12 3.641342 -0.290940 -1.827895
O13 -3.304428 -0.699325 -0.280922
N14 -1.950549 1.189279 -0.192005
O15 -0.105486 2.576610 -0.117414
H16 -2.694581 1.875890 -0.161485
C17 -0.830036 -2.230062 -0.282222
H18 -0.834198 -2.504452 0.777806
H19 -1.638797 -2.750627 -0.795099
H20 0.117714 -2.528093 -0.732730

[5-OH9MOG·2H$_2$O – H]$^{-}$

C1 0.183671 0.130824 0.144620
C2 -1.158164 -0.572236 0.164614
C3 -2.183640 1.383917 -0.128050
C4 0.041526 1.358726 -0.766632
C5 0.510807 -2.048925 -0.128771
N6 -1.146701 2.000003 -0.718909
N7 -2.306991 0.035581 0.158338
O8 1.000093 1.759610 -1.436260
N9 -0.908645 -1.875037 0.160628
N10 -3.268687 2.105465 0.125134
H11 -3.285613 3.090446 -0.095827
H12 -4.089614 1.664041 0.513342
O13 0.966460 -3.191417 -0.291239
N14 1.131037 -0.877388 -0.198350
O15 0.424898 0.711878 1.435319
H16 0.558611 -0.012740 2.063755
H17 3.429559 1.233890 0.681089
O18 3.095946 1.822459 1.386358
H19 2.160397 1.568208 1.457322
H20 3.703728 0.444233 -1.458595
O21 3.720256 -0.052957 -0.633072
H22 2.790673 -0.390351 -0.518372
C23 -1.895871 -2.934817 0.140652
H24 -2.603305 -2.791853 0.959005
H25 -2.434713 -2.942378 -0.810542
H26 -1.381013 -3.885368 0.273479

TS3b^{-}(9MG)



C1 -0.107482 -0.348918 0.477779
C2 -0.083965 1.125414 0.140048
C3 2.151031 1.001025 -0.066238
C4 0.946172 -0.952784 -0.497597

C5 -2.197437 0.343785 0.066383
N6 2.217819 -0.276537 -0.279847
N7 0.993156 1.810551 -0.054038
O8 0.561796 -1.049674 -1.736654
N9 -1.360995 1.519686 0.034917
N10 3.288598 1.721779 0.157537
H11 4.163751 1.280410 -0.085656
H12 3.232703 2.717237 -0.001185
O13 -3.420759 0.442669 -0.130705
N14 -1.478286 -0.746176 0.316811
O15 0.363703 -0.569086 1.803511
H16 -0.320720 -0.269507 2.415153
H17 0.086606 -2.927345 -0.027049
O18 1.186316 -2.397647 0.026895
H19 1.450281 -2.359223 0.960432
H20 -1.290058 -3.526502 -0.952037
O21 -1.073988 -3.226514 -0.058230
H22 -1.478187 -2.261918 0.057827
C23 -1.810548 2.836302 -0.363611
H24 -1.296977 3.593623 0.230936
H25 -1.610767 3.011986 -1.424803
H26 -2.881850 2.909199 -0.180399

[*gem*-9Mdiol – H]$^-$
C1 -0.078234 -0.716028 0.472593
C2 -0.378124 0.742014 0.165644
C3 1.819727 1.160292 -0.002275
C4 1.153417 -1.055595 -0.386522
C5 -2.237932 -0.512558 0.022480
N6 2.193500 -0.073918 -0.209794
N7 0.512352 1.669210 0.009866
N8 -1.703169 0.840875 0.053914
N9 2.754875 2.116866 0.200105
H10 3.726962 1.897284 0.046063
H11 2.471148 3.083601 0.170182
O12 -3.458014 -0.675600 -0.191757
N13 -1.299633 -1.419953 0.231114
O14 0.360547 -0.845073 1.822661
O15 0.717241 -1.110167 -1.721093
H16 1.494712 -0.968600 -2.277279
H17 2.060938 -2.296185 0.796784
O18 1.658793 -2.335289 -0.080713
C19 -2.429506 2.028576 -0.343614
H20 -2.121960 2.872128 0.276823
H21 -2.242942 2.264216 -1.395713
H22 -3.493707 1.848313 -0.196375
H23 -0.425259 -0.783482 2.380478