

Supporting Information

Exploration of the Singlet O₂ Oxidation of 8-Oxoguanine by Guided-Ion Beam Scattering and Density Functional Theory: Changes of Reaction Intermediates, Energetics, and Kinetics upon Protonation/Deprotonation and Hydration

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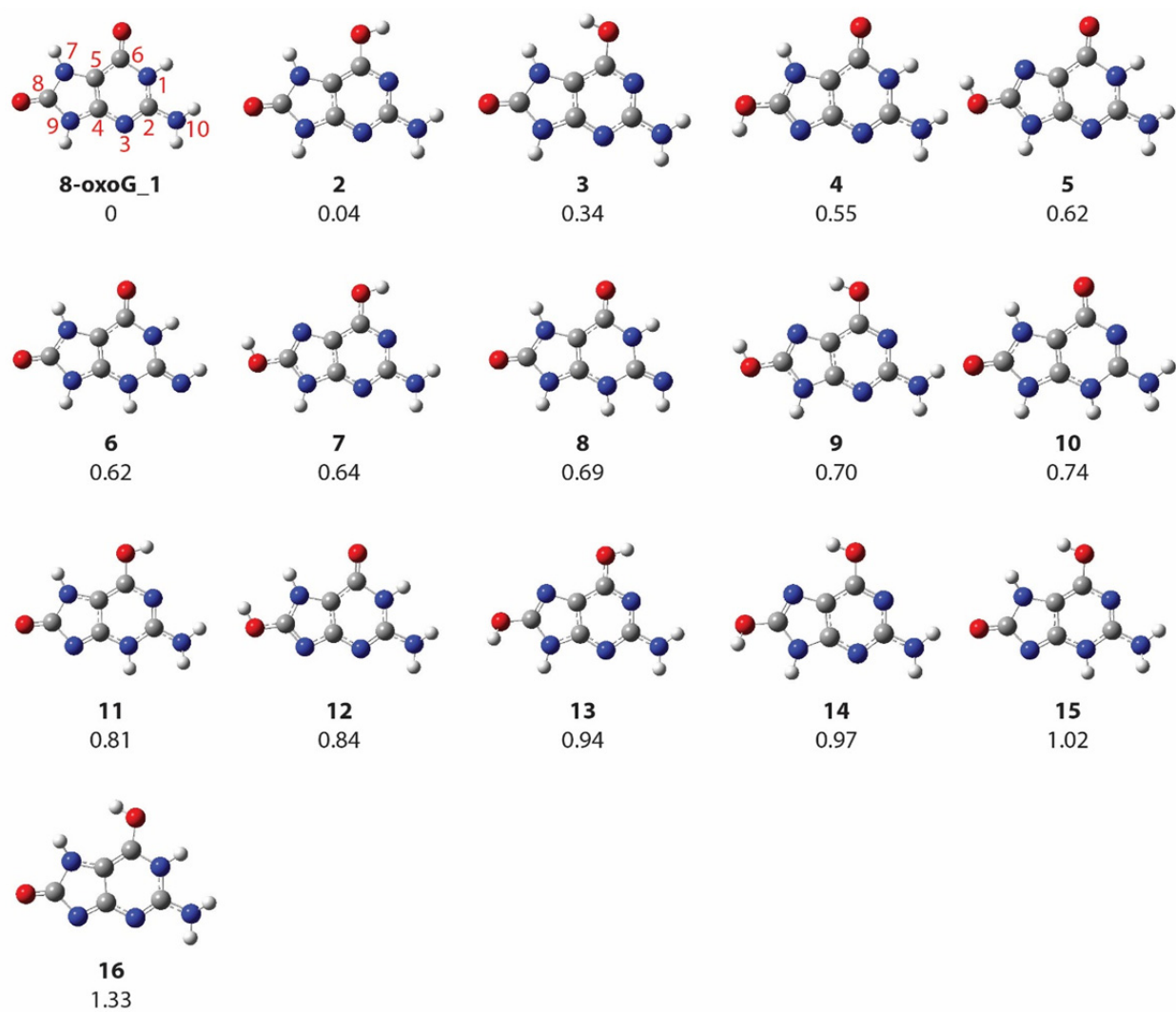


Fig. S1 Stable tautomers/rotamers of 8-oxoG. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).

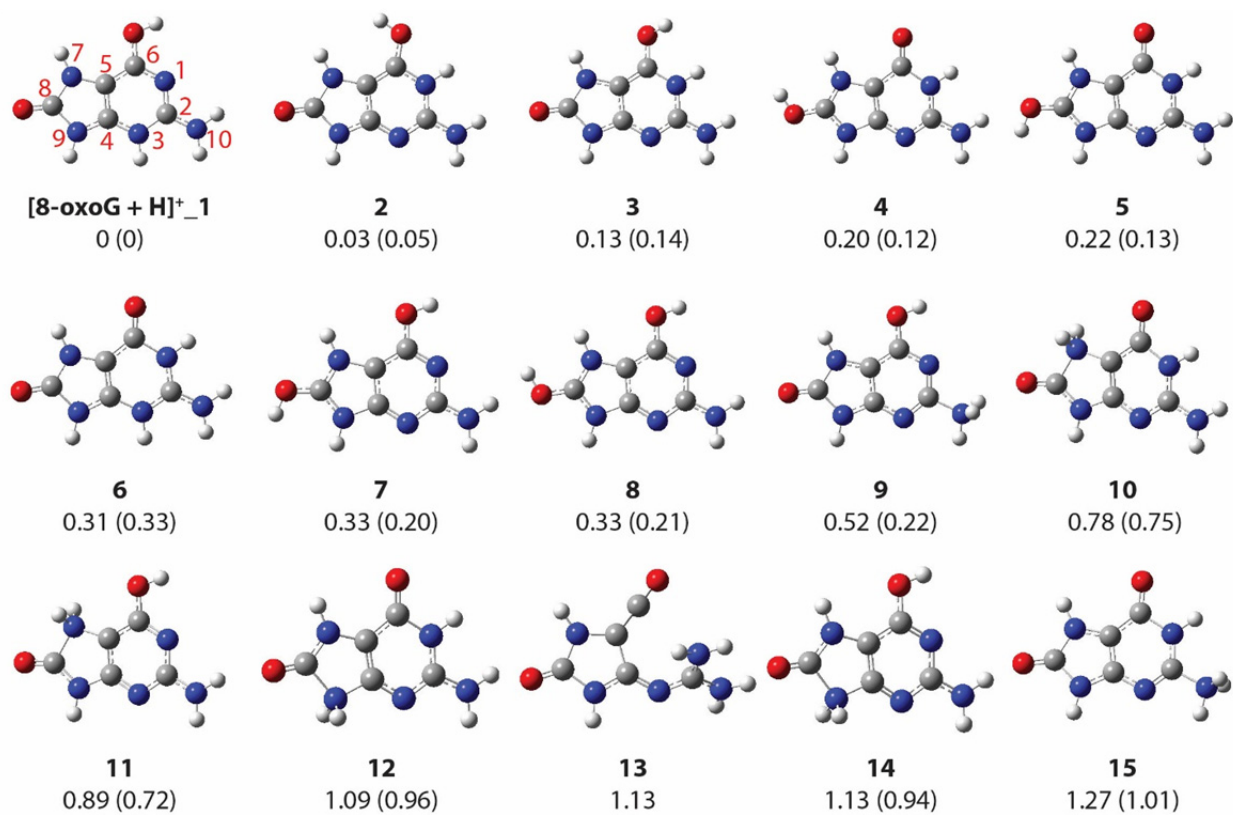


Fig. S2 Stable tautomers/rotamers of $[8\text{-oxoG} + \text{H}]^+$. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p) and MP2/6-311++G(d,p) (presented in parentheses), respectively.

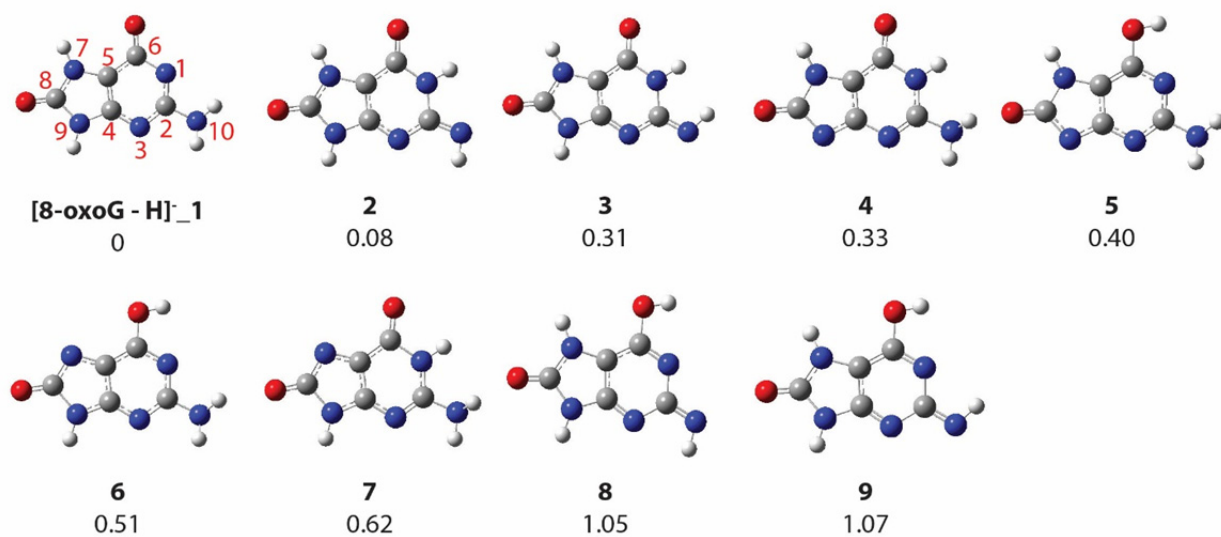


Fig. S3 Stable tautomers/rotamers of [8-oxoG - H]⁻. Relative energies (eV, including thermal corrections at 298 K) were calculated at B3LYP/6-311++G(d,p).

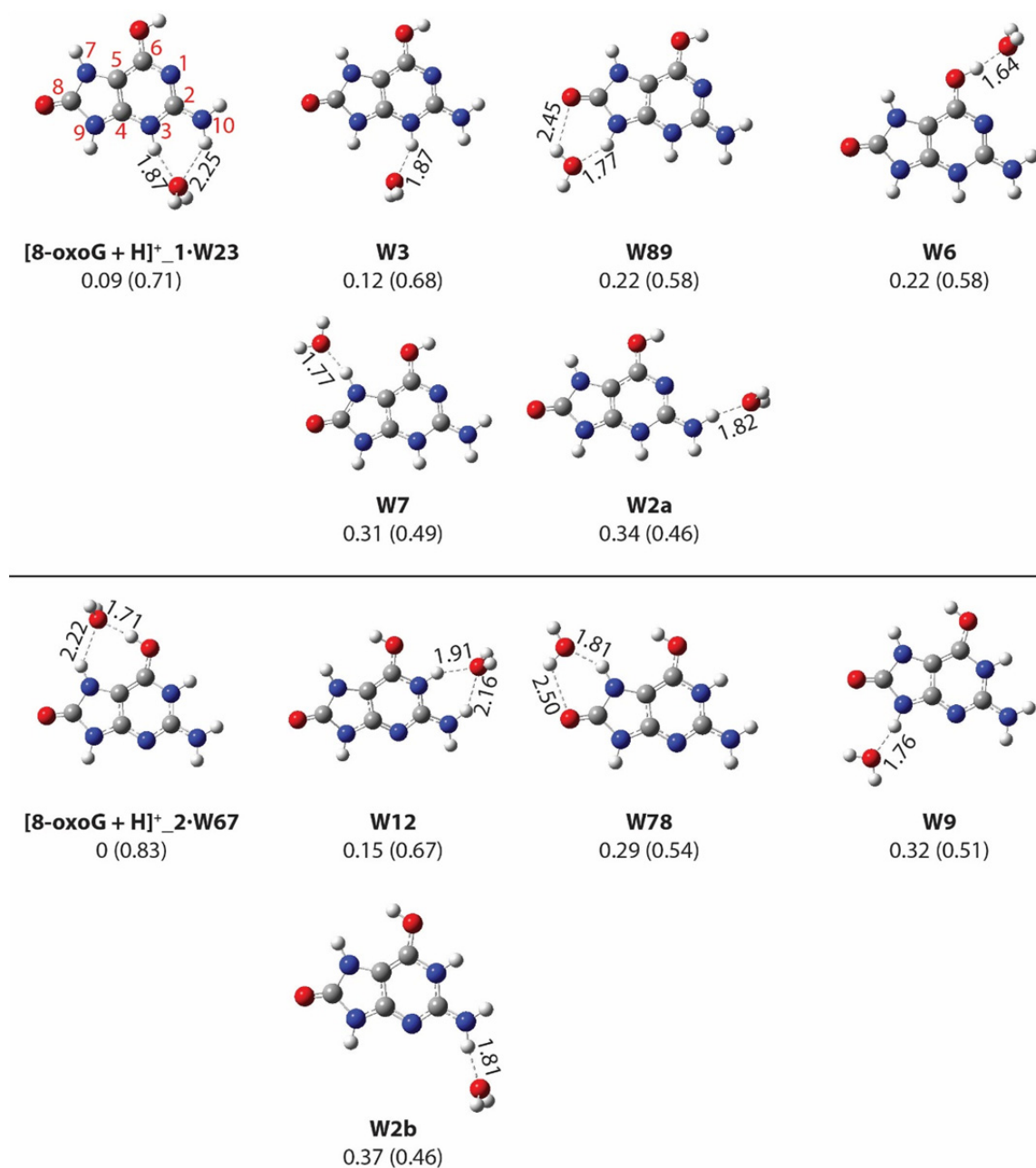


Fig. S4 Stable tautomers of $[8\text{-oxoG} + \text{H}]^+ \cdot \text{W}$. Dashed lines indicate hydrogen bonds, with bond distances shown in Å. Relative energies (eV, including thermal corrections at 298 K) and hydration energies (presented in parentheses) were calculated at B3LYP/6-311++G(d,p).

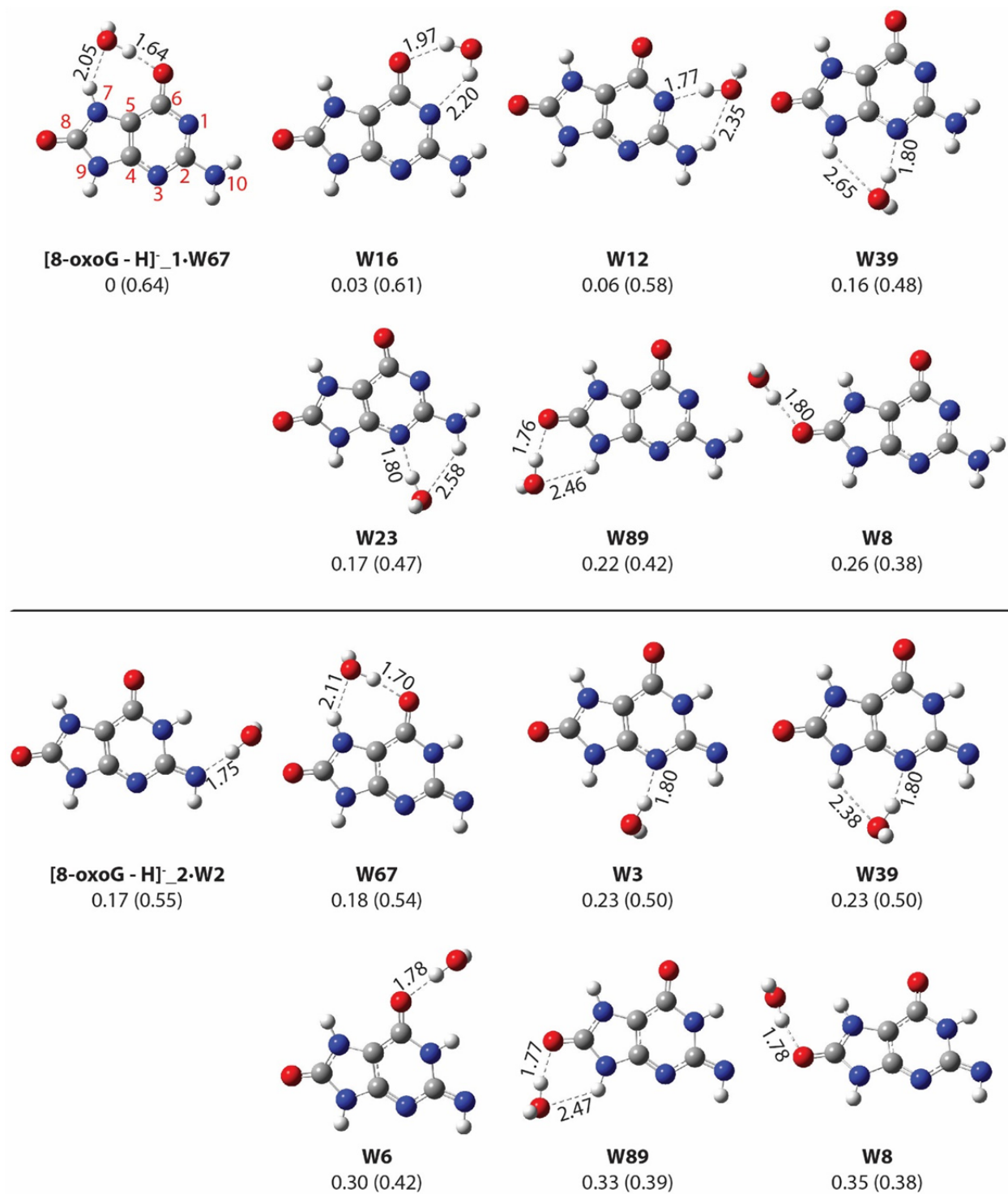


Fig. S5 Stable tautomers of [8-oxoG – H]·W. Dashed lines indicate hydrogen bonds, with bond distances shown in Å. Relative energies (eV, including thermal corrections at 298 K) and hydration energies (presented in parentheses) were calculated at B3LYP/6-311++G(d,p).

**Cartesian coordinates for neutral
8-oxoG in Fig. S1, optimized at
B3LYP/6-311++G(d,p)**

8-oxoG_1

C1 -0.244776 -0.762911 0.000594
 C2 -0.397638 0.608300 0.007490
 C3 0.732277 1.463773 0.002491
 C4 1.984476 -0.691347 -0.001572
 C5 -2.492755 -0.301885 0.000202
 H6 2.779237 1.220834 -0.070913
 H7 -1.729557 -2.291695 -0.008764
 H8 -2.194435 1.789030 0.007767
 O9 0.796922 2.683997 -0.003198
 O10 -3.694707 -0.457329 -0.001938
 N11 -1.765791 0.877756 0.006251
 N12 -1.505634 -1.309138 -0.002180
 N13 0.916094 -1.453228 0.008218
 N14 1.929650 0.674951 -0.001914
 N15 3.226637 -1.272444 -0.063908
 H16 4.009447 -0.782555 0.341721
 H17 3.221392 -2.269809 0.090776
 Zero-point correction= 0.120662 (Hartree/Particle)
 Thermal correction to Energy= 0.130280
 Thermal correction to Enthalpy= 0.131225
 Thermal correction to Gibbs Free Energy= 0.085956
 Sum of electronic and zero-point Energies= -617.870462
 Sum of electronic and thermal Energies= -617.860844
 Sum of electronic and thermal Enthalpies= -617.859900
 Sum of electronic and thermal Free Energies= -617.905169

8-oxoG_2

C1 -0.246778 -0.806252 -0.001105
 C2 -0.368428 0.588094 -0.005869
 C3 0.818646 1.293412 -0.000190
 C4 1.979818 -0.687804 -0.004410
 C5 -2.482434 -0.280772 0.001217
 H6 -1.778098 -2.288934 0.002997
 H7 -2.154147 1.800858 -0.009859
 O8 0.815765 2.641827 0.005997
 O9 -3.687104 -0.401771 0.002056
 N10 -1.731765 0.887384 -0.002868
 N11 -1.525055 -1.313427 0.004532
 N12 0.891047 -1.481135 0.001845
 N13 1.988800 0.656469 0.001259
 N14 3.196174 -1.312701 -0.052919
 H15 4.008168 -0.761972 0.171666
 H16 3.215177 -2.294839 0.167560
 H17 1.740257 2.928234 0.002407
 Zero-point correction= 0.120570 (Hartree/Particle)
 Thermal correction to Energy= 0.130173
 Thermal correction to Enthalpy= 0.131117
 Thermal correction to Gibbs Free Energy= 0.085990
 Sum of electronic and zero-point Energies= -617.869152
 Sum of electronic and thermal Energies= -617.859548
 Sum of electronic and thermal Enthalpies= -617.858604
 Sum of electronic and thermal Free Energies= -617.903731

8-oxoG_3

C1 0.226748 -0.807602 -0.009341
 C2 0.358991 0.586099 0.032625
 C3 -0.826905 1.305665 0.000580
 C4 -1.993964 -0.666678 0.010193
 C5 2.467686 -0.317385 -0.005402
 H6 1.738124 -2.310389 -0.058925
 H7 2.191658 1.732477 0.237399
 O8 -0.900425 2.659272 -0.021262
 O9 3.670284 -0.447104 0.033121
 N10 1.735370 0.870444 -0.013987
 N11 1.500672 -1.330848 -0.048377
 N12 -0.911930 -1.474020 -0.024217
 N13 -1.993796 0.673982 0.008289
 N14 -3.213092 -1.280369 0.074892
 H15 -4.024680 -0.715214 -0.112794
 H16 -3.251292 -2.261987 -0.144151
 H17 -0.028595 3.042847 -0.164523
 Zero-point correction= 0.120058 (Hartree/Particle)
 Thermal correction to Energy= 0.129875
 Thermal correction to Enthalpy= 0.130819
 Thermal correction to Gibbs Free Energy= 0.085239
 Sum of electronic and zero-point Energies= -617.858098
 Sum of electronic and thermal Energies= -617.848281
 Sum of electronic and thermal Enthalpies= -617.847337
 Sum of electronic and thermal Free Energies= -617.892917

8-oxoG_4

C1 -0.262559 -0.784630 0.001092
 C2 -0.360594 0.604173 0.012014
 C3 0.772992 1.456038 0.003170
 C4 1.978128 -0.720447 -0.002168
 C5 -2.335230 -0.326849 0.000201
 H6 2.811521 1.181113 -0.088278
 H7 -2.163678 1.790087 0.012385
 O8 0.842040 2.677687 -0.005882
 O9 -3.670084 -0.393165 -0.003003
 N10 -1.723877 0.882760 0.009609
 N11 -1.515254 -1.352950 -0.004072
 N12 0.912194 -1.471640 0.008951
 N13 1.951053 0.655405 -0.003146
 N14 3.225056 -1.305492 -0.069131
 H15 3.988378 -0.839784 0.399335
 H16 3.197909 -2.304409 0.077916
 H17 -3.910409 -1.329482 -0.011602
 Zero-point correction= 0.120809 (Hartree/Particle)
 Thermal correction to Energy= 0.130309
 Thermal correction to Enthalpy= 0.131253
 Thermal correction to Gibbs Free Energy= 0.086301
 Sum of electronic and zero-point Energies= -617.849999
 Sum of electronic and thermal Energies= -617.840499
 Sum of electronic and thermal Enthalpies= -617.839555
 Sum of electronic and thermal Free Energies= -617.884506

8-oxoG_5

C1 -0.222756 -0.751077 0.000006
 C2 -0.410077 0.625070 0.007791
 C3 0.742610 1.477499 0.002822
 C4 1.995097 -0.695534 -0.002259
 C5 -2.354916 -0.215537 0.001002

H6 2.787412 1.214240 -0.074427
 H7 -1.739347 -2.265761 -0.010530
 O8 0.845041 2.688468 -0.003200
 O9 -3.675615 -0.451853 -0.001260
 N10 -1.765392 0.939205 0.007465
 N11 -1.493599 -1.287744 -0.002993
 N12 0.930735 -1.458163 0.008090
 N13 1.936191 0.671318 -0.003051
 N14 3.244103 -1.270633 -0.066386
 H15 4.012779 -0.781890 0.367689
 H16 3.238207 -2.267242 0.094345
 H17 -4.118470 0.407326 0.000557
 Zero-point correction= 0.120719 (Hartree/Particle)
 Thermal correction to Energy= 0.130214
 Thermal correction to Enthalpy= 0.131158
 Thermal correction to Gibbs Free Energy= 0.086245
 Sum of electronic and zero-point Energies= -617.847709
 Sum of electronic and thermal Energies= -617.838215
 Sum of electronic and thermal Enthalpies= -617.837271
 Sum of electronic and thermal Free Energies= -617.882183

8-oxoG_6

C1 0.261254 -0.761315 0.000003
 C2 0.368500 0.599212 0.000011
 C3 -0.784671 1.440470 0.000001
 C4 -2.142473 -0.711288 -0.000001
 C5 2.492693 -0.248904 0.000000
 H6 -2.824349 1.232465 -0.000031
 H7 1.791068 -2.263307 -0.000022
 H8 2.135225 1.827025 0.000015
 O9 -0.823242 2.659106 -0.000007
 O10 3.694173 -0.393728 -0.000005
 N11 1.736622 0.902214 0.000007
 N12 1.522580 -1.292080 0.000000
 N13 -0.931892 -1.417009 -0.000010
 N14 -1.981795 0.673848 0.000001
 N15 -3.227087 -1.382829 0.000002
 H16 -1.015054 -2.422449 0.000030
 H17 -4.055140 -0.794830 0.000017
 Zero-point correction= 0.119833 (Hartree/Particle)
 Thermal correction to Energy= 0.129764
 Thermal correction to Enthalpy= 0.130708
 Thermal correction to Gibbs Free Energy= 0.084326
 Sum of electronic and zero-point Energies= -617.848060
 Sum of electronic and thermal Energies= -617.838129
 Sum of electronic and thermal Enthalpies= -617.837185
 Sum of electronic and thermal Free Energies= -617.883567

8-oxoG_7

C1 -0.222255 -0.801505 -0.000807
 C2 -0.377021 0.593467 -0.005065
 C3 0.824466 1.301886 -0.000546
 C4 1.990357 -0.687623 -0.005079
 C5 -2.340372 -0.196595 0.000824
 H6 -1.791239 -2.266311 0.001404
 O7 0.841291 2.643470 0.005934
 O8 -3.664653 -0.399362 0.002591
 N9 -1.727533 0.945335 -0.003551
 N10 -1.511509 -1.297698 0.004098

N11 0.913085 -1.487606 0.002135
 N12 1.989872 0.661004 0.000158
 N13 3.218474 -1.295309 -0.055889
 H14 4.016223 -0.731100 0.186494
 H15 3.249438 -2.273875 0.179551
 H16 1.771846 2.910415 0.001896
 H17 -4.087135 0.470156 -0.002167
 Zero-point correction= 0.120773 (Hartree/Particle)
 Thermal correction to Energy= 0.130175
 Thermal correction to Enthalpy= 0.131119
 Thermal correction to Gibbs Free Energy= 0.086508
 Sum of electronic and zero-point Energies= -617.846825
 Sum of electronic and thermal Energies= -617.837424
 Sum of electronic and thermal Enthalpies= -617.836479
 Sum of electronic and thermal Free Energies= -617.881090

8-oxoG_8

C1 0.258818 -0.761324 -0.000433
 C2 0.369137 0.594688 0.000147
 C3 -0.785653 1.443693 -0.000172
 C4 -2.152032 -0.692346 -0.000094
 C5 2.491641 -0.256723 0.000315
 H6 -2.837171 1.220251 -0.000524
 H7 1.788463 -2.268890 -0.001623
 H8 2.134761 1.820620 0.000952
 O9 -0.803653 2.662550 0.000154
 O10 3.693073 -0.403450 0.000498
 N11 1.736461 0.895488 0.000600
 N12 1.519737 -1.297903 -0.000239
 N13 -0.944320 -1.415550 -0.002330
 N14 -1.976738 0.687737 -0.001278
 N15 -3.329131 -1.182965 0.002087
 H16 -0.996351 -2.421395 0.003631
 H17 -3.338587 -2.198965 0.001889
 Zero-point correction= 0.119348 (Hartree/Particle)
 Thermal correction to Energy= 0.129608
 Thermal correction to Enthalpy= 0.130552
 Thermal correction to Gibbs Free Energy= 0.081915
 Sum of electronic and zero-point Energies= -617.845729
 Sum of electronic and thermal Energies= -617.835469
 Sum of electronic and thermal Enthalpies= -617.834525
 Sum of electronic and thermal Free Energies= -617.883162

8-oxoG_9

C1 -0.186393 -0.821030 -0.001145
 C2 -0.360651 0.565315 -0.007054
 C3 0.818005 1.313112 -0.001135
 C4 2.020697 -0.640402 -0.004546
 C5 -2.316724 -0.243158 0.000616
 H6 -1.745677 -2.302887 0.003588
 O7 0.821076 2.659842 0.007004
 O8 -3.637784 -0.463517 0.002973
 N9 -1.714937 0.907891 -0.005049
 N10 -1.473640 -1.331919 0.004582
 N11 0.964939 -1.476315 0.002804
 N12 1.994189 0.708103 0.000587
 N13 3.262222 -1.215679 -0.052744
 H14 4.046997 -0.624343 0.166078
 H15 3.325975 -2.194174 0.174592

H16 -4.076731 0.397362 -0.002770
 H17 -0.095924 2.965858 0.007023
 Zero-point correction= 0.120716 (Hartree/Particle)
 Thermal correction to Energy= 0.130179
 Thermal correction to Enthalpy= 0.131123
 Thermal correction to Gibbs Free Energy= 0.086394
 Sum of electronic and zero-point Energies= -617.844727
 Sum of electronic and thermal Energies= -617.835264
 Sum of electronic and thermal Enthalpies= -617.834320
 Sum of electronic and thermal Free Energies= -617.879049

8-oxoG_10

C1 -0.259361 -0.760088 -0.006885
 C2 -0.381115 0.591548 0.006702
 C3 0.773343 1.463257 -0.002366
 C4 2.070841 -0.514688 0.008714
 C5 -2.493425 -0.292559 0.002493
 H6 -1.769464 -2.295073 0.013512
 H7 -2.155776 1.792327 0.022344
 O8 0.704685 2.681510 -0.021938
 O9 -3.694606 -0.449784 0.006321
 N10 -1.749800 0.870188 0.010497
 N11 -1.513164 -1.321404 -0.011396
 N12 0.971674 -1.370827 0.013816
 N13 2.003233 0.773734 0.032051
 N14 3.292225 -1.156767 -0.069727
 H15 4.065579 -0.512338 0.022129
 H16 3.404223 -2.000229 0.476011
 H17 1.083918 -2.327779 -0.287700
 Zero-point correction= 0.119960 (Hartree/Particle)
 Thermal correction to Energy= 0.129860
 Thermal correction to Enthalpy= 0.130804
 Thermal correction to Gibbs Free Energy= 0.084886
 Sum of electronic and zero-point Energies= -617.843553
 Sum of electronic and thermal Energies= -617.833654
 Sum of electronic and thermal Enthalpies= -617.832709
 Sum of electronic and thermal Free Energies= -617.878627

8-oxoG_11

C1 -0.369656 -0.814094 0.001912
 C2 -0.428964 0.609032 0.008571
 C3 0.738719 1.314276 0.000364
 C4 1.999660 -0.617021 -0.000933
 C5 -2.483866 -0.374179 0.001177
 H6 -2.237883 1.762057 0.011570
 O7 0.752239 2.663181 -0.006810
 O8 -3.689055 -0.475234 0.000231
 N9 -1.783289 0.864096 0.007079
 N10 -1.526616 -1.413241 -0.003553
 N11 0.875038 -1.401340 -0.008579
 N12 1.951754 0.687748 0.013573
 N13 3.211278 -1.264249 -0.064307
 H14 4.003424 -0.656434 0.083772
 H15 3.290402 -2.166362 0.381751
 H16 0.929521 -2.408335 -0.089912
 H17 1.676555 2.946313 -0.010586
 Zero-point correction= 0.120125 (Hartree/Particle)
 Thermal correction to Energy= 0.129841
 Thermal correction to Enthalpy= 0.130786
 Thermal correction to Gibbs Free Energy= 0.085387

Sum of electronic and zero-point Energies= -617.840920
 Sum of electronic and thermal Energies= -617.831204
 Sum of electronic and thermal Enthalpies= -617.830260
 Sum of electronic and thermal Free Energies= -617.875659

8-oxoG_12

C1 -0.249618 -0.799292 0.001114
 C2 -0.364328 0.587104 0.012701
 C3 0.753727 1.457453 0.003241
 C4 1.990584 -0.699303 -0.002123
 C5 -2.330569 -0.384222 -0.000185
 H6 2.796377 1.215145 -0.088835
 H7 -2.155559 1.760544 0.020297
 O8 0.799167 2.681215 -0.006297
 O9 -3.660430 -0.556899 -0.001535
 N10 -1.731507 0.845426 0.009493
 N11 -1.490222 -1.387792 -0.004968
 N12 0.936840 -1.466768 0.008617
 N13 1.943660 0.677173 -0.002609
 N14 3.246438 -1.264593 -0.069163
 H15 4.002453 -0.788246 0.400431
 H16 3.234393 -2.264256 0.075234
 H17 -4.122796 0.287729 -0.022547
 Zero-point correction= 0.119724 (Hartree/Particle)
 Thermal correction to Energy= 0.129808
 Thermal correction to Enthalpy= 0.130752
 Thermal correction to Gibbs Free Energy= 0.084086
 Sum of electronic and zero-point Energies= -617.839919
 Sum of electronic and thermal Energies= -617.829835
 Sum of electronic and thermal Enthalpies= -617.828891
 Sum of electronic and thermal Free Energies= -617.875557

8-oxoG_13

C1 -0.232723 -0.789186 0.004393
 C2 -0.367938 0.606245 -0.002054
 C3 0.845382 1.298196 0.002311
 C4 1.980492 -0.709780 -0.004763
 C5 -2.349741 -0.138547 -0.001739
 H6 -1.799395 -2.227847 -0.113254
 O7 0.881744 2.637557 0.008507
 O8 -3.691267 -0.248296 -0.061667
 N9 -1.708436 0.982818 0.002351
 N10 -1.529075 -1.264299 0.012594
 N11 0.892000 -1.494173 0.006111
 N12 2.000149 0.639415 0.002419
 N13 3.199228 -1.333815 -0.060552
 H14 4.007124 -0.780347 0.172531
 H15 3.219513 -2.313825 0.169528
 H16 1.815740 2.892397 0.002378
 H17 -3.996693 -0.995661 0.464742
 Zero-point correction= 0.119845 (Hartree/Particle)
 Thermal correction to Energy= 0.129658
 Thermal correction to Enthalpy= 0.130602
 Thermal correction to Gibbs Free Energy= 0.084999
 Sum of electronic and zero-point Energies= -617.836149
 Sum of electronic and thermal Energies= -617.826336
 Sum of electronic and thermal Enthalpies= -617.825392
 Sum of electronic and thermal Free Energies= -617.870995

8-oxoG_14

C1 -0.195786 -0.811023 0.002526
 C2 -0.352105 0.575434 -0.005650
 C3 0.836781 1.309670 0.001275
 C4 2.012721 -0.660497 -0.004036
 C5 -2.326027 -0.188546 -0.001061
 H6 -1.752034 -2.269131 -0.104591
 O7 0.853547 2.654247 0.009350
 O8 -3.665713 -0.307687 -0.054245
 N9 -1.695666 0.942141 0.000832
 N10 -1.490765 -1.301781 0.011613
 N11 0.946566 -1.483345 0.006040
 N12 2.004355 0.689052 0.003038
 N13 3.246414 -1.250458 -0.056340
 H14 4.040107 -0.668402 0.154892
 H15 3.300587 -2.230567 0.166069
 H16 -3.960097 -1.093212 0.420188
 H17 -0.061066 2.969324 0.008002
 Zero-point correction= 0.119906 (Hartree/Particle)
 Thermal correction to Energy= 0.129732
 Thermal correction to Enthalpy= 0.130676
 Thermal correction to Gibbs Free Energy= 0.085093
 Sum of electronic and zero-point Energies= -617.835053
 Sum of electronic and thermal Energies= -617.825227
 Sum of electronic and thermal Enthalpies= -617.824283
 Sum of electronic and thermal Free Energies= -617.869866

8-oxoG_15

C1 -0.347776 -0.819031 -0.012015
 C2 -0.419608 0.602580 0.031491
 C3 0.743473 1.324324 0.002961
 C4 2.014447 -0.591277 0.006999
 C5 -2.466720 -0.413056 -0.003774
 H6 -2.268904 1.690914 0.237808
 O7 0.826279 2.675074 -0.024216
 O8 -3.669825 -0.522877 0.039253
 N9 -1.785211 0.846033 -0.021213
 N10 -1.499306 -1.432291 -0.045116
 N11 0.899120 -1.392936 -0.032309
 N12 1.955471 0.709573 0.034183
 N13 3.233124 -1.224926 -0.040765
 H14 4.014501 -0.604450 0.113904
 H15 3.319217 -2.126584 0.404725
 H16 0.966090 -2.396643 -0.140738
 H17 -0.047819 3.059780 -0.153428
 Zero-point correction= 0.119927 (Hartree/Particle)
 Thermal correction to Energy= 0.129712
 Thermal correction to Enthalpy= 0.130657
 Thermal correction to Gibbs Free Energy= 0.085117
 Sum of electronic and zero-point Energies= -617.833101
 Sum of electronic and thermal Energies= -617.823315
 Sum of electronic and thermal Enthalpies= -617.822371
 Sum of electronic and thermal Free Energies= -617.867910

8-oxoG_16

C1 -0.339902 -0.859918 0.014687
 C2 -0.436131 0.595088 -0.020711
 C3 0.698139 1.321376 -0.003575
 C4 1.929718 -0.747259 -0.003095
 C5 -2.472354 -0.414941 0.007140

H6 2.743198 1.163123 -0.167155
 H7 -2.265234 1.691442 -0.247547
 O8 0.881851 2.665257 0.006587
 O9 -3.676007 -0.504556 -0.046022
 N10 -1.788519 0.852579 0.044525
 N11 -1.516884 -1.432888 0.044050
 N12 0.865338 -1.495973 0.034285
 N13 1.901050 0.627210 -0.011326
 N14 3.174766 -1.326060 -0.090116
 H15 3.946519 -0.867354 0.371753
 H16 3.149367 -2.327715 0.039231
 H17 0.052314 3.114734 0.202591
 Zero-point correction= 0.119200 (Hartree/Particle)
 Thermal correction to Energy= 0.129243
 Thermal correction to Enthalpy= 0.130187
 Thermal correction to Gibbs Free Energy= 0.084160
 Sum of electronic and zero-point Energies= -617.822107
 Sum of electronic and thermal Energies= -617.812065
 Sum of electronic and thermal Enthalpies= -617.811120
 Sum of electronic and thermal Free Energies= -617.857147

**Cartesian coordinates for protonated
8-oxoG in Fig. S2, optimized at
B3LYP/6-311++G(d,p)**

[8-oxoG + H]⁺_1

C1 -0.296319 -0.796479 0.000002
 C2 -0.401439 0.584625 0.000012
 C3 0.782814 1.318509 0.000002
 C4 2.053560 -0.607050 0.000013
 C5 -2.520214 -0.272369 0.000002
 H6 -1.809383 -2.301206 -0.000012
 H7 -2.167042 1.809409 0.000018
 O8 0.726593 2.637952 -0.000016
 O9 -3.704614 -0.419935 -0.000002
 N10 -1.755367 0.887517 0.000011
 N11 -1.534369 -1.328467 -0.000002
 N12 0.922335 -1.403340 -0.000002
 N13 1.973898 0.708998 0.000033
 N14 3.253024 -1.206114 -0.000136
 H15 4.073913 -0.618998 0.000195
 H16 3.379884 -2.205329 0.000632
 H17 1.622397 3.011760 -0.000023
 H18 0.997343 -2.413348 -0.000175
 Zero-point correction= 0.132779 (Hartree/Particle)
 Thermal correction to Energy= 0.142861
 Thermal correction to Enthalpy= 0.143805
 Thermal correction to Gibbs Free Energy= 0.097751
 Sum of electronic and zero-point Energies= -618.211365
 Sum of electronic and thermal Energies= -618.201283
 Sum of electronic and thermal Enthalpies= -618.200339
 Sum of electronic and thermal Free Energies= -618.246393

[8-oxoG + H]⁺_2

C1 -0.272244 -0.809459 -0.000057
 C2 -0.410836 0.611058 0.000114
 C3 0.744264 1.333792 -0.000002
 C4 1.971300 -0.750732 0.000024
 C5 -2.509951 -0.304897 -0.000011
 H6 2.778022 1.171669 -0.000023
 H7 -1.752250 -2.311449 -0.000269
 H8 -2.238705 1.779080 0.000946
 O9 0.951901 2.647912 -0.000036
 O10 -3.694524 -0.447180 0.000145
 N11 -1.771114 0.885403 -0.000067
 N12 -1.517558 -1.326935 -0.000182
 N13 0.864403 -1.484171 -0.000087
 N14 1.926920 0.619684 0.000044
 N15 3.163297 -1.359123 0.000084
 H16 4.042332 -0.866925 0.000281
 H17 3.176425 -2.368547 0.000094
 H18 0.138331 3.167746 -0.000846
 Zero-point correction= 0.132251 (Hartree/Particle)
 Thermal correction to Energy= 0.142690
 Thermal correction to Enthalpy= 0.143634
 Thermal correction to Gibbs Free Energy= 0.096530
 Sum of electronic and zero-point Energies= -618.210747
 Sum of electronic and thermal Energies= -618.200308
 Sum of electronic and thermal Enthalpies= -618.199364
 Sum of electronic and thermal Free Energies= -618.246468

[8-oxoG + H]⁺_3

C1 -0.269517 -0.821097 -0.006977
 C2 -0.408887 0.598142 -0.005601
 C3 0.731986 1.335537 0.003794
 C4 1.974971 -0.747102 0.003111
 C5 -2.504843 -0.301982 0.002345
 H6 2.787335 1.153307 -0.126326
 H7 -1.754566 -2.317934 0.009089
 H8 -2.194269 1.791540 -0.013379
 O9 0.737897 2.666935 -0.048529
 O10 -3.688589 -0.447435 0.004367
 N11 -1.759631 0.880549 0.006235
 N12 -1.513308 -1.335040 -0.001942
 N13 0.874441 -1.486574 0.007614
 N14 1.928729 0.629484 -0.005116
 N15 3.171512 -1.349772 -0.002794
 H16 4.048158 -0.857198 0.056568
 H17 3.187489 -2.359302 0.001815
 H18 1.476940 3.082063 0.417527
 Zero-point correction= 0.132146 (Hartree/Particle)
 Thermal correction to Energy= 0.142497
 Thermal correction to Enthalpy= 0.143441
 Thermal correction to Gibbs Free Energy= 0.096832
 Sum of electronic and zero-point Energies= -618.207012
 Sum of electronic and thermal Energies= -618.196661
 Sum of electronic and thermal Enthalpies= -618.195717
 Sum of electronic and thermal Free Energies= -618.242327

[8-oxoG + H]⁺_4

C1 0.187493 -0.758575 0.000006
 C2 0.338425 0.607782 0.000008
 C3 -0.800919 1.474228 0.000005
 C4 -2.032313 -0.699936 0.000003
 C5 2.369498 -0.277912 -0.000003
 H6 -2.840990 1.215390 -0.000079
 H7 1.728597 -2.272115 -0.000025
 H8 2.116524 1.812467 0.000033
 O9 -0.837358 2.683037 -0.000005
 O10 3.658206 -0.513913 0.000017
 N11 1.712319 0.883491 0.000005
 N12 1.481302 -1.289269 0.000000
 N13 -0.943084 -1.460005 0.000018
 N14 -1.982891 0.674508 0.000009
 N15 -3.236230 -1.292165 -0.000104
 H16 -4.102979 -0.779981 0.000384
 H17 -3.269968 -2.300105 0.000162
 H18 4.209009 0.281919 -0.000181
 Zero-point correction= 0.132963 (Hartree/Particle)
 Thermal correction to Energy= 0.143061
 Thermal correction to Enthalpy= 0.144006
 Thermal correction to Gibbs Free Energy= 0.097845
 Sum of electronic and zero-point Energies= -618.204053
 Sum of electronic and thermal Energies= -618.193954
 Sum of electronic and thermal Enthalpies= -618.193010
 Sum of electronic and thermal Free Energies= -618.239170

[8-oxoG + H]⁺_5

C1 -0.187830 -0.754252 0.000008

C2 -0.339884 0.611119 0.000011
 C3 0.804938 1.473556 0.000005
 C4 2.031059 -0.705671 0.000004
 C5 -2.372273 -0.267916 -0.000002
 H6 2.843973 1.206850 -0.000070
 H7 -1.701115 -2.277568 -0.000005
 H8 -2.142947 1.801654 0.000003
 O9 0.849337 2.680998 -0.000005
 O10 -3.682053 -0.314796 -0.000007
 N11 -1.710449 0.884633 0.000003
 N12 -1.485311 -1.288205 0.000002
 N13 0.938942 -1.461909 0.000017
 N14 1.984522 0.668082 0.000005
 N15 3.233503 -1.301407 -0.000085
 H16 4.101329 -0.791051 0.000317
 H17 3.265350 -2.309288 0.000119
 H18 -4.049379 -1.209600 -0.000012
 Zero-point correction= 0.132847 (Hartree/Particle)
 Thermal correction to Energy= 0.143029
 Thermal correction to Enthalpy= 0.143973
 Thermal correction to Gibbs Free Energy= 0.097609
 Sum of electronic and zero-point Energies= -618.203509
 Sum of electronic and thermal Energies= -618.193328
 Sum of electronic and thermal Enthalpies= -618.192384
 Sum of electronic and thermal Free Energies= -618.238748

[8-oxoG + H]⁺₆

C1 0.296859 -0.744218 0.000005
 C2 0.440275 0.615904 0.000002
 C3 -0.682474 1.493480 0.000002
 C4 -2.066379 -0.615669 0.000006
 C5 2.536855 -0.296181 -0.000002
 H6 -2.759368 1.301522 0.000005
 H7 1.771161 -2.299410 0.000010
 H8 2.226337 1.798134 -0.000006
 O9 -0.743559 2.692728 -0.000006
 O10 3.719281 -0.471942 -0.000005
 N11 1.799837 0.882405 -0.000004
 N12 1.524662 -1.319727 0.000004
 N13 -0.939937 -1.367574 0.000015
 N14 -1.930711 0.714729 0.000021
 N15 -3.267861 -1.202499 -0.000065
 H16 -4.115825 -0.655113 0.000106
 H17 -3.374575 -2.205840 0.000147
 H18 -1.006247 -2.376811 -0.000048
 Zero-point correction= 0.132033 (Hartree/Particle)
 Thermal correction to Energy= 0.142536
 Thermal correction to Enthalpy= 0.143480
 Thermal correction to Gibbs Free Energy= 0.096477
 Sum of electronic and zero-point Energies= -618.200354
 Sum of electronic and thermal Energies= -618.189851
 Sum of electronic and thermal Enthalpies= -618.188907
 Sum of electronic and thermal Free Energies= -618.235910

[8-oxoG + H]⁺₇

C1 -0.190150 -0.794395 0.000006
 C2 -0.308242 0.588677 -0.000019
 C3 0.896303 1.304575 0.000003
 C4 2.023214 -0.712654 0.000001

C5 -2.362103 -0.249596 -0.000001
 H6 -1.749119 -2.275573 0.000031
 H7 -2.104552 1.810305 -0.000046
 O8 0.868919 2.633978 0.000016
 O9 -3.671727 -0.262782 -0.000004
 N10 -1.677983 0.891715 -0.000020
 N11 -1.505686 -1.292721 0.000020
 N12 0.916852 -1.495738 0.000029
 N13 2.034553 0.646507 0.000020
 N14 3.215237 -1.326244 -0.000173
 H15 4.061176 -0.780086 0.000425
 H16 3.263118 -2.332115 0.000397
 H17 1.778771 2.971776 0.000016
 H18 -4.061862 -1.148157 -0.000004
 Zero-point correction= 0.133092 (Hartree/Particle)
 Thermal correction to Energy= 0.142983
 Thermal correction to Enthalpy= 0.143928
 Thermal correction to Gibbs Free Energy= 0.098317
 Sum of electronic and zero-point Energies= -618.199088
 Sum of electronic and thermal Energies= -618.189197
 Sum of electronic and thermal Enthalpies= -618.188253
 Sum of electronic and thermal Free Energies= -618.233864

[8-oxoG + H]⁺₈

C1 -0.190049 -0.797479 -0.000002
 C2 -0.307488 0.586713 -0.000003
 C3 0.893412 1.306111 0.000001
 C4 2.024468 -0.707775 0.000001
 C5 -2.360281 -0.259905 0.000001
 H6 -1.775705 -2.268747 0.000016
 H7 -2.080435 1.820892 -0.000028
 O8 0.861275 2.636679 0.000002
 O9 -3.653766 -0.462765 -0.000013
 N10 -1.681174 0.891141 -0.000003
 N11 -1.501527 -1.293142 0.000002
 N12 0.920463 -1.493576 0.000003
 N13 2.033465 0.652078 0.000003
 N14 3.217575 -1.318772 -0.000024
 H15 4.062821 -0.771541 0.000070
 H16 3.266594 -2.324710 0.000065
 H17 1.770252 2.976851 0.000001
 H18 -4.185575 0.345859 0.000110
 Zero-point correction= 0.133155 (Hartree/Particle)
 Thermal correction to Energy= 0.143001
 Thermal correction to Enthalpy= 0.143945
 Thermal correction to Gibbs Free Energy= 0.098437
 Sum of electronic and zero-point Energies= -618.198993
 Sum of electronic and thermal Energies= -618.189147
 Sum of electronic and thermal Enthalpies= -618.188203
 Sum of electronic and thermal Free Energies= -618.233712

[8-oxoG + H]⁺₉

C1 -0.278857 -0.816109 -0.000308
 C2 -0.425859 0.584330 0.001380
 C3 0.732934 1.348839 0.000004
 C4 1.900532 -0.580367 -0.002082
 C5 -2.515437 -0.337325 0.000366
 H6 -1.758782 -2.339107 -0.002066
 H7 -2.211950 1.763874 0.002274

O8 0.664115 2.675905 -0.000597
 O9 -3.702078 -0.479616 0.000436
 N10 -1.772727 0.854506 0.001641
 N11 -1.523133 -1.356363 -0.000996
 N12 0.905691 -1.439245 -0.002258
 N13 1.930640 0.728594 -0.001394
 N14 3.250332 -1.229641 0.002210
 H15 3.755586 -1.027072 0.872177
 H16 3.126919 -2.244572 -0.084177
 H17 1.552322 3.062214 -0.001473
 H18 3.824119 -0.886819 -0.776032
 Zero-point correction= 0.134461 (Hartree/Particle)
 Thermal correction to Energy= 0.144357
 Thermal correction to Enthalpy= 0.145301
 Thermal correction to Gibbs Free Energy= 0.098155
 Sum of electronic and zero-point Energies= -618.191900
 Sum of electronic and thermal Energies= -618.182004
 Sum of electronic and thermal Enthalpies= -618.181060
 Sum of electronic and thermal Free Energies= -618.228205

[8-oxoG + H]⁺₁₀

C1 -0.219715 -0.748224 -0.000005
 C2 -0.339938 0.617503 0.000000
 C3 0.800168 1.469585 -0.000005
 C4 2.011105 -0.705602 -0.000002
 C5 -2.506778 -0.433627 0.000001
 H6 2.848328 1.194051 0.000031
 H7 -1.666545 -2.331834 -0.000008
 H8 -2.049518 1.512762 -0.825196
 O9 0.852998 2.677624 -0.000006
 O10 -3.682220 -0.494636 0.000002
 N11 -1.746862 0.979173 0.000010
 N12 -1.494538 -1.332711 -0.000008
 N13 0.897980 -1.451228 -0.000012
 N14 1.985215 0.660182 -0.000004
 N15 3.189398 -1.334589 0.000052
 H16 4.073647 -0.851234 -0.000155
 H17 3.189964 -2.343991 -0.000071
 H18 -2.049508 1.512742 0.825233
 Zero-point correction= 0.133754 (Hartree/Particle)
 Thermal correction to Energy= 0.143558
 Thermal correction to Enthalpy= 0.144502
 Thermal correction to Gibbs Free Energy= 0.098602
 Sum of electronic and zero-point Energies= -618.182229
 Sum of electronic and thermal Energies= -618.172426
 Sum of electronic and thermal Enthalpies= -618.171481
 Sum of electronic and thermal Free Energies= -618.217381

[8-oxoG + H]⁺₁₁

C1 -0.224326 -0.789124 -0.000006
 C2 -0.307994 0.595598 0.000007
 C3 0.896175 1.297775 -0.000004
 C4 2.002017 -0.716715 0.000000
 C5 -2.506521 -0.412149 -0.000001
 H6 -1.720106 -2.326937 -0.000024
 H7 -2.004735 1.526420 -0.826460
 O8 0.879754 2.626621 -0.000014
 O9 -3.683085 -0.432054 -0.000002
 N10 -1.706532 0.993925 0.000025

N11 -1.519865 -1.332911 -0.000014
 N12 0.874027 -1.488371 -0.000012
 N13 2.037367 0.635797 -0.000005
 N14 3.170256 -1.362814 0.000021
 H15 4.033713 -0.842967 0.000005
 H16 3.187678 -2.370546 0.000007
 H17 1.791941 2.959418 -0.000025
 H18 -2.004722 1.526375 0.826543
 Zero-point correction= 0.133991 (Hartree/Particle)
 Thermal correction to Energy= 0.143593
 Thermal correction to Enthalpy= 0.144538
 Thermal correction to Gibbs Free Energy= 0.099154
 Sum of electronic and zero-point Energies= -618.178332
 Sum of electronic and thermal Energies= -618.168730
 Sum of electronic and thermal Enthalpies= -618.167786
 Sum of electronic and thermal Free Energies= -618.213170

[8-oxoG + H]⁺₁₂

C1 -0.164564 -0.758251 0.000000
 C2 -0.380055 0.577548 -0.000008
 C3 0.748252 1.472090 -0.000005
 C4 2.053452 -0.655578 -0.000004
 C5 -2.557122 -0.177701 -0.000001
 H6 2.796383 1.283588 0.000092
 H7 -1.645563 -2.001210 -0.826949
 H8 -2.120985 1.840784 -0.000016
 O9 0.743810 2.679159 0.000001
 O10 -3.715222 -0.390954 -0.000001
 N11 -1.752404 0.895985 -0.000003
 N12 -1.484672 -1.415013 0.000006
 N13 0.974114 -1.437279 -0.000015
 N14 1.957426 0.712185 0.000006
 N15 3.267965 -1.221352 0.000095
 H16 4.123437 -0.689505 -0.000432
 H17 3.326810 -2.228445 -0.000178
 H18 -1.645564 -2.001193 0.826973
 Zero-point correction= 0.133043 (Hartree/Particle)
 Thermal correction to Energy= 0.143020
 Thermal correction to Enthalpy= 0.143965
 Thermal correction to Gibbs Free Energy= 0.097881
 Sum of electronic and zero-point Energies= -618.171381
 Sum of electronic and thermal Energies= -618.161403
 Sum of electronic and thermal Enthalpies= -618.160458
 Sum of electronic and thermal Free Energies= -618.206542

[8-oxoG + H]⁺₁₃

C1 -0.225179 -0.594683 -0.066651
 C2 -0.611744 0.813174 -0.035287
 C3 0.183248 1.864986 -0.238343
 C4 2.124511 -0.735996 0.101138
 C5 -2.546532 -0.431063 0.030485
 H6 3.285117 0.373815 1.395052
 H7 -1.462794 -2.279378 -0.051920
 H8 -2.596428 1.658754 0.184221
 O9 0.865594 2.779524 -0.368515
 O10 -3.683807 -0.786740 0.113907
 N11 -2.026746 0.849431 -0.014044
 N12 -1.394832 -1.269478 -0.033714
 N13 0.920869 -1.215112 -0.202998

N14 2.345559 0.108035 1.135064
 N15 3.158711 -1.139317 -0.640094
 H16 4.118439 -0.960922 -0.386113
 H17 2.976789 -1.742519 -1.428853
 H18 1.653826 0.174564 1.866927
 Zero-point correction= 0.130166 (Hartree/Particle)
 Thermal correction to Energy= 0.141637
 Thermal correction to Enthalpy= 0.142581
 Thermal correction to Gibbs Free Energy= 0.092434
 Sum of electronic and zero-point Energies= -618.171220
 Sum of electronic and thermal Energies= -618.159749
 Sum of electronic and thermal Enthalpies= -618.158805
 Sum of electronic and thermal Free Energies= -618.208953

H17 -3.078768 -2.249521 -0.000054
 H18 -3.822077 -1.012301 0.834054
 Zero-point correction= 0.133719 (Hartree/Particle)
 Thermal correction to Energy= 0.143607
 Thermal correction to Enthalpy= 0.144551
 Thermal correction to Gibbs Free Energy= 0.098564
 Sum of electronic and zero-point Energies= -618.164530
 Sum of electronic and thermal Energies= -618.154641
 Sum of electronic and thermal Enthalpies= -618.153697
 Sum of electronic and thermal Free Energies= -618.199685

[8-oxoG + H]⁺_14

C1 -0.166749 -0.796718 0.000003
 C2 -0.345308 0.562034 0.000003
 C3 0.843487 1.309165 0.000001
 C4 2.044499 -0.661757 0.000000
 C5 -2.540323 -0.157456 -0.000001
 H6 -1.683082 -1.997666 -0.826834
 H7 -2.082254 1.848084 -0.000005
 O8 0.769668 2.635005 -0.000001
 O9 -3.704742 -0.339721 -0.000004
 N10 -1.716307 0.903400 0.000003
 N11 -1.507020 -1.415762 0.000001
 N12 0.948034 -1.471309 0.000000
 N13 2.006971 0.690148 0.000000
 N14 3.246970 -1.251307 0.000005
 H15 4.082314 -0.688044 -0.000027
 H16 3.318076 -2.256111 -0.000022
 H17 1.664449 3.011324 -0.000002
 H18 -1.683087 -1.997662 0.826839
 Zero-point correction= 0.133263 (Hartree/Particle)
 Thermal correction to Energy= 0.143016
 Thermal correction to Enthalpy= 0.143960
 Thermal correction to Gibbs Free Energy= 0.098414
 Sum of electronic and zero-point Energies= -618.169322
 Sum of electronic and thermal Energies= -618.159569
 Sum of electronic and thermal Enthalpies= -618.158625
 Sum of electronic and thermal Free Energies= -618.204171

[8-oxoG + H]⁺_15

C1 0.280135 -0.763703 0.000003
 C2 0.464269 0.607845 0.000003
 C3 -0.636395 1.523089 0.000000
 C4 -1.925367 -0.580093 0.000002
 C5 2.530898 -0.364757 -0.000001
 H6 -2.717399 1.353627 0.000002
 H7 1.716137 -2.339897 0.000002
 H8 2.265984 1.748798 -0.000002
 O9 -0.657452 2.727656 0.000003
 O10 3.715633 -0.535930 -0.000006
 N11 1.814675 0.844491 0.000003
 N12 1.511251 -1.350890 0.000001
 N13 -0.929995 -1.389615 0.000007
 N14 -1.888219 0.767526 -0.000010
 N15 -3.263205 -1.236738 -0.000002
 H16 -3.822109 -1.012222 -0.834015

**Cartesian coordinates for deprotonated
8-oxoG in Fig. S3, optimized at
B3LYP/6-311++G(d,p)**

[8-oxoG – H]⁻_1

C1 -0.202556 -0.777137 -0.008885
 C2 -0.341296 0.588519 -0.012938
 C3 0.813517 1.437744 -0.002628
 C4 2.000600 -0.598367 -0.015307
 C5 -2.453302 -0.300447 0.004804
 H6 -1.730378 -2.290890 -0.004171
 H7 -2.133645 1.780964 -0.004199
 O8 0.754397 2.683011 0.012331
 O9 -3.675900 -0.443746 0.010095
 N10 -1.722015 0.863478 -0.001580
 N11 -1.491677 -1.313892 0.003799
 N12 0.953667 -1.452932 -0.008865
 N13 2.008972 0.728937 -0.003809
 N14 3.262482 -1.218073 -0.071863
 H15 3.992624 -0.615562 0.280584
 H16 3.261641 -2.143135 0.334339
 Zero-point correction= 0.107675 (Hartree/Particle)
 Thermal correction to Energy= 0.116958
 Thermal correction to Enthalpy= 0.117902
 Thermal correction to Gibbs Free Energy= 0.073151
 Sum of electronic and zero-point Energies= -617.345274
 Sum of electronic and thermal Energies= -617.335991
 Sum of electronic and thermal Enthalpies= -617.335047
 Sum of electronic and thermal Free Energies= -617.379798

[8-oxoG – H]⁻_2

C1 -0.196242 -0.780985 -0.000143
 C2 -0.330350 0.601501 -0.000096
 C3 0.817115 1.422939 -0.000056
 C4 2.074053 -0.777776 -0.000005
 C5 -2.450159 -0.262024 0.000049
 H6 2.855357 1.127682 0.000231
 H7 -1.744551 -2.261320 -0.000004
 H8 -2.122616 1.811296 0.000115
 O9 0.879127 2.664003 0.000123
 O10 -3.672399 -0.394090 0.000150
 N11 -1.711749 0.894148 0.000052
 N12 -1.497691 -1.286012 -0.000105
 N13 0.908497 -1.510564 -0.000140
 N14 1.975957 0.631452 -0.000348
 N15 3.278717 -1.268470 0.000379
 H16 3.195377 -2.282766 0.000115
 Zero-point correction= 0.107227 (Hartree/Particle)
 Thermal correction to Energy= 0.116691
 Thermal correction to Enthalpy= 0.117636
 Thermal correction to Gibbs Free Energy= 0.072097
 Sum of electronic and zero-point Energies= -617.342346
 Sum of electronic and thermal Energies= -617.332882
 Sum of electronic and thermal Enthalpies= -617.331938
 Sum of electronic and thermal Free Energies= -617.377476

[8-oxoG – H]⁻_3

C1 -0.205483 -0.782690 -0.000012
 C2 -0.333150 0.604067 -0.000055

C3 0.818063 1.410425 -0.000006
 C4 2.063281 -0.822737 0.000000
 C5 -2.457137 -0.249199 0.000005
 H6 2.836935 1.122624 0.000126
 H7 -1.761415 -2.252519 0.000059
 H8 -2.120959 1.822528 -0.000072
 O9 0.909299 2.650665 0.000036
 O10 -3.679998 -0.372339 0.000018
 N11 -1.712990 0.904183 -0.000025
 N12 -1.511388 -1.277877 0.000015
 N13 0.884396 -1.525419 0.000010
 N14 1.973182 0.599637 -0.000011
 N15 3.213622 -1.433280 -0.000002
 H16 3.969833 -0.749129 -0.000042
 Zero-point correction= 0.106601 (Hartree/Particle)
 Thermal correction to Energy= 0.116184
 Thermal correction to Enthalpy= 0.117128
 Thermal correction to Gibbs Free Energy= 0.071319
 Sum of electronic and zero-point Energies= -617.334012
 Sum of electronic and thermal Energies= -617.324429
 Sum of electronic and thermal Enthalpies= -617.323485
 Sum of electronic and thermal Free Energies= -617.369295

[8-oxoG – H]⁻_4

C1 -0.316765 -0.809240 -0.003532
 C2 -0.418486 0.600944 0.015563
 C3 0.688478 1.453031 0.003106
 C4 1.941370 -0.691638 -0.008887
 C5 -2.459291 -0.399998 0.000490
 H6 2.742189 1.211196 -0.143855
 H7 -2.240220 1.736576 0.026606
 O8 0.778735 2.694084 -0.011476
 O9 -3.689905 -0.497567 0.000689
 N10 -1.783757 0.840834 0.013157
 N11 -1.511728 -1.409963 -0.009962
 N12 0.900553 -1.463499 0.004411
 N13 1.899090 0.674795 0.003630
 N14 3.230729 -1.257180 -0.078303
 H15 3.876491 -0.872300 0.601653
 H16 3.154847 -2.261107 0.030922
 Zero-point correction= 0.107007 (Hartree/Particle)
 Thermal correction to Energy= 0.116507
 Thermal correction to Enthalpy= 0.117451
 Thermal correction to Gibbs Free Energy= 0.072077
 Sum of electronic and zero-point Energies= -617.333411
 Sum of electronic and thermal Energies= -617.323911
 Sum of electronic and thermal Enthalpies= -617.322967
 Sum of electronic and thermal Free Energies= -617.368341

[8-oxoG – H]⁻_5

C1 -0.320908 -0.850374 -0.000443
 C2 -0.397045 0.580658 -0.005834
 C3 0.774201 1.279912 -0.002557
 C4 1.936701 -0.686635 -0.017652
 C5 -2.453962 -0.383700 0.006615
 H6 -2.197985 1.746711 -0.101452
 O7 0.805799 2.654136 0.008891
 O8 -3.684697 -0.436225 -0.017408
 N9 -1.751203 0.857136 0.039813

N10 -1.539481 -1.413104 0.012829
 N11 0.872894 -1.486304 -0.001300
 N12 1.967616 0.654994 -0.014496
 N13 3.188863 -1.322368 -0.080088
 H14 3.930538 -0.769912 0.326044
 H15 3.147585 -2.268094 0.273117
 H16 1.746302 2.876358 -0.007657
 Zero-point correction= 0.107054 (Hartree/Particle)
 Thermal correction to Energy= 0.116450
 Thermal correction to Enthalpy= 0.117394
 Thermal correction to Gibbs Free Energy= 0.072428
 Sum of electronic and zero-point Energies= -617.330867
 Sum of electronic and thermal Energies= -617.321471
 Sum of electronic and thermal Enthalpies= -617.320527
 Sum of electronic and thermal Free Energies= -617.365493

[8-oxoG – H]_6

C1 -0.282161 -0.807263 -0.007977
 C2 -0.442603 0.607040 -0.008335
 C3 0.763851 1.289887 -0.003011
 C4 1.944887 -0.683410 -0.014419
 C5 -2.480871 -0.169062 0.004232
 H6 -1.825108 -2.258746 -0.005165
 O7 0.825465 2.653653 0.009352
 O8 -3.700400 -0.372380 0.010123
 N9 -1.766838 0.977849 -0.000442
 N10 -1.547889 -1.291188 0.002408
 N11 0.870121 -1.482606 -0.008486
 N12 1.950018 0.649906 -0.005491
 N13 3.199335 -1.319977 -0.074626
 H14 3.935592 -0.754886 0.325020
 H15 3.167093 -2.254315 0.309486
 H16 1.770056 2.856716 -0.001630
 Zero-point correction= 0.107170 (Hartree/Particle)
 Thermal correction to Energy= 0.116358
 Thermal correction to Enthalpy= 0.117302
 Thermal correction to Gibbs Free Energy= 0.072915
 Sum of electronic and zero-point Energies= -617.326324
 Sum of electronic and thermal Energies= -617.317136
 Sum of electronic and thermal Enthalpies= -617.316192
 Sum of electronic and thermal Free Energies= -617.360580

[8-oxoG – H]_7

C1 -0.279005 -0.756080 -0.007417
 C2 -0.472904 0.634347 0.011394
 C3 0.688228 1.468044 0.001308
 C4 1.950807 -0.695652 -0.009289
 C5 -2.493597 -0.198927 0.004298
 H6 2.733292 1.207996 -0.121863
 H7 -1.778359 -2.259661 -0.018409
 O8 0.823193 2.692251 -0.006417
 O9 -3.711705 -0.427886 0.005951
 N10 -1.804385 0.966710 0.016914
 N11 -1.533706 -1.283292 -0.011682
 N12 0.891978 -1.454173 0.003941
 N13 1.886995 0.666189 -0.011904
 N14 3.240398 -1.265031 -0.070405
 H15 3.864675 -0.914748 0.649186
 H16 3.158363 -2.271711 0.005003

Zero-point correction= 0.106817 (Hartree/Particle)
 Thermal correction to Energy= 0.116151
 Thermal correction to Enthalpy= 0.117096
 Thermal correction to Gibbs Free Energy= 0.072272
 Sum of electronic and zero-point Energies= -617.322429
 Sum of electronic and thermal Energies= -617.313095
 Sum of electronic and thermal Enthalpies= -617.312151
 Sum of electronic and thermal Free Energies= -617.356974

[8-oxoG – H]_8

C1 0.204955 -0.808838 0.012168
 C2 0.314313 0.586173 0.064581
 C3 -0.900274 1.254894 0.003022
 C4 -2.087645 -0.773416 0.000290
 C5 2.448016 -0.244211 -0.009762
 H6 1.791352 -2.253969 -0.066605
 H7 2.106250 1.802133 0.190403
 O8 -0.922814 2.628619 -0.027773
 O9 3.672576 -0.345446 0.009029
 N10 1.692625 0.908151 -0.009928
 N11 1.521697 -1.285442 -0.031024
 N12 -0.888953 -1.520726 -0.026216
 N13 -2.047800 0.628927 -0.014172
 N14 -3.252669 -1.356444 0.029080
 H15 -3.078014 -2.361073 0.030778
 H16 -1.868166 2.838645 -0.060594
 Zero-point correction= 0.106720 (Hartree/Particle)
 Thermal correction to Energy= 0.116180
 Thermal correction to Enthalpy= 0.117125
 Thermal correction to Gibbs Free Energy= 0.071619
 Sum of electronic and zero-point Energies= -617.306701
 Sum of electronic and thermal Energies= -617.297240
 Sum of electronic and thermal Enthalpies= -617.296296
 Sum of electronic and thermal Free Energies= -617.341802

[8-oxoG – H]_9

C1 0.219072 -0.817619 0.012556
 C2 0.312649 0.581881 0.070773
 C3 -0.906843 1.233908 0.002642
 C4 -2.061756 -0.827921 0.000259
 C5 2.455115 -0.224413 -0.010210
 H6 1.822012 -2.241791 -0.073901
 H7 2.090901 1.813713 0.214239
 O8 -0.952235 2.607458 -0.031649
 O9 3.680550 -0.308502 0.011342
 N10 1.686583 0.921153 -0.010848
 N11 1.542811 -1.275947 -0.034771
 N12 -0.857679 -1.548568 -0.029270
 N13 -2.046160 0.584829 -0.016478
 N14 -3.184788 -1.488066 0.032920
 H15 -3.934764 -0.797523 0.044786
 H16 -1.899458 2.805135 -0.069656
 Zero-point correction= 0.106686 (Hartree/Particle)
 Thermal correction to Energy= 0.116134
 Thermal correction to Enthalpy= 0.117078
 Thermal correction to Gibbs Free Energy= 0.071642
 Sum of electronic and zero-point Energies= -617.306115
 Sum of electronic and thermal Energies= -617.296667
 Sum of electronic and thermal Enthalpies= -617.295723
 Sum of electronic and thermal Free Energies= -617.341159

Cartesian coordinates for monohydrated protonated 8-oxoG in Fig. S4, optimized at B3LYP/6-311++G(d,p)

[8-oxoG + H]⁺_1-W23

C1 -0.259424 -0.558437 -0.000010
 C2 -1.017827 0.601357 0.000003
 C3 -0.331864 1.813491 0.000006
 C4 1.701322 0.729802 -0.000012
 C5 -2.461624 -1.170461 -0.000001
 H6 -0.863522 -2.604176 -0.000022
 H7 -3.157070 0.822068 0.000018
 O8 -1.016362 2.946288 0.000016
 O9 -3.431203 -1.870082 -0.000001
 N10 -2.351857 0.213705 0.000008
 N11 -1.093114 -1.620525 -0.000012
 N12 1.095403 -0.510570 -0.000018
 N13 1.004236 1.853187 0.000002
 N14 3.040766 0.760759 -0.000031
 H15 3.498191 1.659160 0.000006
 H16 3.588754 -0.088292 0.000039
 H17 -0.405460 3.700144 0.000017
 H18 1.685401 -1.350708 -0.000043
 O19 3.291881 -2.315674 0.000028
 H20 3.623828 -2.796448 -0.769162
 H21 3.623822 -2.796411 0.769243
 Zero-point correction= 0.158067 (Hartree/Particle)
 Thermal correction to Energy= 0.171028
 Thermal correction to Enthalpy= 0.171972
 Thermal correction to Gibbs Free Energy= 0.118971
 Sum of electronic and zero-point Energies= -694.673689
 Sum of electronic and thermal Energies= -694.660728
 Sum of electronic and thermal Enthalpies= -694.659784
 Sum of electronic and thermal Free Energies= -694.712785

[8-oxoG + H]⁺_1-W3

C1 0.284018 0.364622 -0.000051
 C2 0.456081 -1.009978 0.000005
 C3 -0.696336 -1.790512 0.000041
 C4 -2.040538 0.085632 -0.000044
 C5 2.527347 -0.039586 -0.000033
 H6 1.682805 1.952660 -0.000087
 H7 2.287092 -2.138603 0.000047
 O8 -0.591085 -3.109833 0.000098
 O9 3.705792 0.163778 -0.000035
 N10 1.825679 -1.241133 0.000012
 N11 1.493003 0.959310 -0.000067
 N12 -0.950035 0.926077 -0.000080
 N13 -1.911535 -1.229128 0.000019
 N14 -3.266213 0.634895 -0.000075
 H15 -4.063449 0.017249 -0.000057
 H16 -3.424310 1.629041 -0.000139
 H17 -1.474404 -3.511194 0.000118
 H18 -1.017971 1.950908 -0.000144
 O19 -0.246065 3.648789 0.000140
 H20 -0.229313 4.233306 0.768782
 H21 -0.229306 4.233539 -0.768324

Zero-point correction= 0.157508 (Hartree/Particle)
 Thermal correction to Energy= 0.170792
 Thermal correction to Enthalpy= 0.171736
 Thermal correction to Gibbs Free Energy= 0.117508
 Sum of electronic and zero-point Energies= -694.673087
 Sum of electronic and thermal Energies= -694.659803
 Sum of electronic and thermal Enthalpies= -694.658859
 Sum of electronic and thermal Free Energies= -694.713087

[8-oxoG + H]⁺_1-W89

C1 0.127177 0.420532 0.000025
 C2 -0.309870 -0.897480 0.000006
 C3 -1.682018 -1.120362 -0.000011
 C4 -2.116221 1.145834 0.000002
 C5 1.967617 -0.895881 0.000024
 H6 2.145867 1.223582 0.000050
 H7 0.864061 -2.699447 -0.000014
 O8 -2.142547 -2.360187 -0.000028
 O9 3.127150 -1.210947 0.000017
 N10 0.829578 -1.690729 0.000011
 N11 1.467903 0.445092 0.000044
 N12 -0.767254 1.447265 0.000023
 N13 -2.549225 -0.098813 -0.000013
 N14 -2.993917 2.161219 -0.000003
 H15 -3.977234 1.935441 -0.000020
 H16 -2.725110 3.131656 0.000005
 H17 -3.112868 -2.353619 -0.000040
 H18 -0.445302 2.407471 0.000028
 O19 3.840637 1.724415 -0.000099
 H20 4.462604 2.458664 0.000271
 H21 4.356348 0.905911 -0.000096
 Zero-point correction= 0.156783 (Hartree/Particle)
 Thermal correction to Energy= 0.170336
 Thermal correction to Enthalpy= 0.171281
 Thermal correction to Gibbs Free Energy= 0.116461
 Sum of electronic and zero-point Energies= -694.669592
 Sum of electronic and thermal Energies= -694.656039
 Sum of electronic and thermal Enthalpies= -694.655094
 Sum of electronic and thermal Free Energies= -694.709914

[8-oxoG + H]⁺_1-W6

C1 1.121460 0.782489 -0.001766
 C2 0.541749 -0.470050 0.004613
 C3 -0.855889 -0.551764 0.008431
 C4 -1.022314 1.753887 0.000427
 C5 2.810203 -0.755235 -0.001637
 H6 3.178989 1.359441 -0.010675
 H7 1.486075 -2.399646 0.008909
 O8 -1.424488 -1.727128 0.013938
 O9 3.917829 -1.206040 -0.003402
 N10 1.578196 -1.394773 0.004396
 N11 2.465647 0.644072 -0.005607
 N12 0.352339 1.907309 -0.004238
 N13 -1.595553 0.569610 0.007105
 N14 -1.780576 2.863493 0.000671
 H15 -2.782384 2.745950 -0.005286
 H16 -1.405881 3.797709 -0.019403
 H17 -2.425379 -1.697628 0.009405
 H18 0.775781 2.826658 -0.007009

O19 -4.054424 -1.918808 -0.019568
 H20 -4.487923 -2.370806 -0.752601
 H21 -4.562231 -2.129821 0.772230
 Zero-point correction= 0.156336 (Hartree/Particle)
 Thermal correction to Energy= 0.170166
 Thermal correction to Enthalpy= 0.171110
 Thermal correction to Gibbs Free Energy= 0.115146
 Sum of electronic and zero-point Energies= -694.669809
 Sum of electronic and thermal Energies= -694.655979
 Sum of electronic and thermal Enthalpies= -694.655035
 Sum of electronic and thermal Free Energies= -694.710998

[8-oxoG + H]⁺_1-W7

C1 -0.455651 -1.044080 -0.000001
 C2 0.143443 0.207935 -0.000008
 C3 -0.702099 1.314882 -0.000009
 C4 -2.580861 -0.025773 0.000007
 C5 1.806237 -1.338810 -0.000010
 H6 0.418845 -2.989234 0.000003
 H7 2.256837 0.724485 -0.000009
 O8 -0.186387 2.532725 -0.000019
 O9 2.860254 -1.907510 -0.000009
 N10 1.512853 0.011063 -0.000017
 N11 0.508664 -1.982773 -0.000003
 N12 -1.811125 -1.173671 0.000007
 N13 -2.034549 1.172604 -0.000001
 N14 -3.917594 -0.155998 0.000014
 H15 -4.473574 0.685765 0.000016
 H16 -4.392638 -1.043767 0.000026
 H17 -0.899591 3.190549 -0.000017
 H18 -2.242996 -2.089456 0.000010
 O19 3.781128 1.628397 0.000042
 H20 4.004167 2.564886 -0.000094
 H21 4.614833 1.144381 0.000075
 Zero-point correction= 0.156085 (Hartree/Particle)
 Thermal correction to Energy= 0.170142
 Thermal correction to Enthalpy= 0.171086
 Thermal correction to Gibbs Free Energy= 0.114006
 Sum of electronic and zero-point Energies= -694.666724
 Sum of electronic and thermal Energies= -694.652668
 Sum of electronic and thermal Enthalpies= -694.651724
 Sum of electronic and thermal Free Energies= -694.708804

[8-oxoG + H]⁺_1-W2a

C1 -0.909085 -0.794260 -0.000002
 C2 -1.009886 0.585091 -0.000001
 C3 0.179560 1.312636 -0.000002
 C4 1.448715 -0.616763 -0.000007
 C5 -3.131820 -0.264526 0.000004
 H6 -2.428720 -2.293935 0.000001
 H7 -2.773676 1.815271 0.000005
 O8 0.126911 2.634820 0.000000
 O9 -4.318227 -0.408123 0.000007
 N10 -2.364771 0.892584 0.000003
 N11 -2.151019 -1.322363 0.000001
 N12 0.306093 -1.405564 -0.000005
 N13 1.366873 0.704542 -0.000007
 N14 2.635813 -1.222267 -0.000012
 H15 3.500247 -0.668000 -0.000004

H16 2.726401 -2.225809 -0.000013
 H17 1.026754 2.998189 0.000002
 H18 0.376894 -2.415394 -0.000004
 O19 5.202440 -0.034633 0.000012
 H20 5.733600 0.195908 -0.770097
 H21 5.733679 0.195673 0.770138
 Zero-point correction= 0.156620 (Hartree/Particle)
 Thermal correction to Energy= 0.170347
 Thermal correction to Enthalpy= 0.171291
 Thermal correction to Gibbs Free Energy= 0.115851
 Sum of electronic and zero-point Energies= -694.665513
 Sum of electronic and thermal Energies= -694.651786
 Sum of electronic and thermal Enthalpies= -694.650842
 Sum of electronic and thermal Free Energies= -694.706283

[8-oxoG + H]⁺_2-W67

C1 -0.440947 -1.150653 -0.000007
 C2 0.305668 0.056780 -0.000029
 C3 -0.400000 1.226942 -0.000056
 C4 -2.424507 -0.104716 0.000025
 C5 1.794048 -1.674266 -0.000016
 H6 -2.297490 1.976144 -0.000029
 H7 0.235047 -3.150811 0.000006
 H8 2.432997 0.351525 0.000079
 O9 0.020769 2.475258 -0.000105
 O10 2.796924 -2.326332 0.000017
 N11 1.649060 -0.287155 -0.000058
 N12 0.453271 -2.163182 -0.000014
 N13 -1.762506 -1.253601 0.000018
 N14 -1.777986 1.105402 -0.000011
 N15 -3.765767 -0.117436 0.000065
 H16 -4.331747 0.715347 0.000078
 H17 -4.227108 -1.014748 0.000091
 H18 1.008847 2.551158 -0.000293
 O19 2.715603 2.553109 0.000104
 H20 3.167702 2.921197 -0.770885
 H21 3.167303 2.921189 0.771330
 Zero-point correction= 0.158062 (Hartree/Particle)
 Thermal correction to Energy= 0.170947
 Thermal correction to Enthalpy= 0.171891
 Thermal correction to Gibbs Free Energy= 0.119299
 Sum of electronic and zero-point Energies= -694.677078
 Sum of electronic and thermal Energies= -694.664193
 Sum of electronic and thermal Enthalpies= -694.663249
 Sum of electronic and thermal Free Energies= -694.715842

[8-oxoG + H]⁺_2-W12

C1 0.891502 -0.833594 -0.000008
 C2 0.830368 0.590539 -0.000019
 C3 -0.415927 1.145582 -0.000052
 C4 -1.336130 -1.080224 -0.000029
 C5 3.037801 -0.022466 0.000028
 H6 -2.434069 0.675197 -0.000010
 H7 2.570301 -2.112897 0.000036
 H8 2.480330 2.002082 0.000100
 O9 -0.788872 2.425750 -0.000059
 O10 4.232398 0.003974 0.000080
 N11 2.141188 1.052611 -0.000022
 N12 2.200475 -1.171354 0.000009

N13 -0.138055 -1.660694 -0.000005
 N14 -1.485194 0.282078 -0.000044
 N15 -2.442541 -1.830564 -0.000080
 H16 -3.363643 -1.411785 -0.000123
 H17 -2.336635 -2.833382 0.000009
 H18 -0.042256 3.037133 -0.000151
 O19 -4.335575 0.517404 0.000121
 H20 -4.857080 0.781482 0.768891
 H21 -4.857349 0.781581 -0.768432
 Zero-point correction= 0.157519 (Hartree/Particle)
 Thermal correction to Energy= 0.170874
 Thermal correction to Enthalpy= 0.171818
 Thermal correction to Gibbs Free Energy= 0.117774
 Sum of electronic and zero-point Energies= -694.671880
 Sum of electronic and thermal Energies= -694.658524
 Sum of electronic and thermal Enthalpies= -694.657580
 Sum of electronic and thermal Free Energies= -694.711625

[8-oxoG + H]⁺_2·W78

C1 -0.447037 -1.001321 0.000023
 C2 0.097520 0.317120 0.000094
 C3 -0.798777 1.343693 0.000037
 C4 -2.576639 -0.295343 -0.000033
 C5 1.835896 -1.143861 0.000057
 H6 -2.792887 1.777731 -0.000052
 H7 0.546811 -2.862989 -0.000055
 H8 2.217515 0.905821 0.000221
 O9 -0.607469 2.660209 0.000034
 O10 2.938162 -1.619789 0.000014
 N11 1.474674 0.197656 0.000145
 N12 0.599792 -1.852671 0.000013
 N13 -1.731565 -1.318604 -0.000030
 N14 -2.137464 1.003751 -0.000011
 N15 -3.895827 -0.530810 -0.000063
 H16 -4.593186 0.195875 -0.000065
 H17 -4.201607 -1.492559 -0.000088
 H18 0.326933 2.905667 -0.000114
 O19 3.989169 1.264084 -0.000278
 H20 4.413358 0.395026 -0.000439
 H21 4.691112 1.922418 0.000997
 Zero-point correction= 0.156532 (Hartree/Particle)
 Thermal correction to Energy= 0.170267
 Thermal correction to Enthalpy= 0.171211
 Thermal correction to Gibbs Free Energy= 0.115564
 Sum of electronic and zero-point Energies= -694.667193
 Sum of electronic and thermal Energies= -694.653458
 Sum of electronic and thermal Enthalpies= -694.652514
 Sum of electronic and thermal Free Energies= -694.708161

[8-oxoG + H]⁺_2·W9

C1 0.183458 0.361428 -0.000002
 C2 -0.354129 -0.964780 -0.000009
 C3 -1.709970 -1.076043 -0.000019
 C4 -1.840640 1.337637 0.000016
 C5 1.926260 -1.103719 0.000011
 H6 -3.442842 0.002862 0.000011
 H7 2.219481 1.018257 0.000046
 H8 0.735064 -2.840231 0.000009
 O9 -2.499823 -2.149894 -0.000031

O10 3.046236 -1.526581 0.000060
 N11 0.727637 -1.832018 -0.000008
 N12 1.522092 0.254089 -0.000008
 N13 -0.523496 1.483223 -0.000007
 N14 -2.433715 0.101275 0.000007
 N15 -2.623971 2.425760 0.000030
 H16 -3.630349 2.389657 0.000041
 H17 -2.173140 3.328394 0.000029
 H18 -2.012380 -2.982859 -0.000051
 O19 3.697885 1.966495 -0.000042
 H20 4.542838 1.501971 0.000046
 H21 3.897249 2.908350 -0.000112
 Zero-point correction= 0.155552 (Hartree/Particle)
 Thermal correction to Energy= 0.169950
 Thermal correction to Enthalpy= 0.170894
 Thermal correction to Gibbs Free Energy= 0.113282
 Sum of electronic and zero-point Energies= -694.666887
 Sum of electronic and thermal Energies= -694.652489
 Sum of electronic and thermal Enthalpies= -694.651545
 Sum of electronic and thermal Free Energies= -694.709157

[8-oxoG + H]⁺_2·W2b

C1 0.390202 -0.645177 0.000006
 C2 1.207032 0.525982 0.000001
 C3 0.551422 1.719062 -0.000007
 C4 -1.544497 0.497973 0.000004
 C5 2.590869 -1.298883 0.000006
 H6 -1.300990 2.569714 0.000009
 H7 0.952073 -2.678811 0.000016
 H8 3.374176 0.649992 0.000006
 O9 1.014439 2.968425 -0.000016
 O10 3.556495 -2.002197 0.000009
 N11 2.529415 0.099485 -0.000003
 N12 1.228203 -1.705702 0.000008
 N13 -0.927723 -0.684021 0.000003
 N14 -0.827546 1.673163 -0.000001
 N15 -2.873437 0.555519 0.000017
 H16 -3.372130 1.431354 -0.000050
 H17 -3.428670 -0.308899 0.000020
 H18 1.978225 3.019442 -0.000023
 O19 -4.713389 -1.585980 -0.000026
 H20 -5.067371 -2.044219 -0.770077
 H21 -5.068239 -2.043391 0.770121
 Zero-point correction= 0.155988 (Hartree/Particle)
 Thermal correction to Energy= 0.170153
 Thermal correction to Enthalpy= 0.171097
 Thermal correction to Gibbs Free Energy= 0.114117
 Sum of electronic and zero-point Energies= -694.664779
 Sum of electronic and thermal Energies= -694.650614
 Sum of electronic and thermal Enthalpies= -694.649670
 Sum of electronic and thermal Free Energies= -694.706649

Cartesian coordinates for monohydrated deprotonated 8-oxoG in Fig. S5, optimized at B3LYP/6-311++G(d,p)

[8-oxoG - H]⁻_1·W67

C1 -0.393207 -1.110208 0.012926
 C2 0.247982 0.109354 -0.008625
 C3 -0.525830 1.307982 -0.029070
 C4 -2.376030 -0.131334 0.025780
 C5 1.872952 -1.496938 -0.013418
 H6 0.457780 -3.078968 0.032774
 H7 2.347808 0.576830 -0.032503
 O8 -0.029741 2.470298 -0.067621
 O9 2.945991 -2.096159 -0.012294
 N10 1.632661 -0.145591 -0.030461
 N11 0.599032 -2.083610 0.006160
 N12 -1.716271 -1.306928 0.029484
 N13 -1.887425 1.104588 -0.008186
 N14 -3.774531 -0.233897 0.099212
 H15 -4.236025 0.590652 -0.257266
 H16 -4.126731 -1.101240 -0.279971
 O17 2.609384 2.613341 -0.019021
 H18 1.605569 2.636514 -0.075661
 H19 2.817060 3.061290 0.805093
 Zero-point correction= 0.132821 (Hartree/Particle)
 Thermal correction to Energy= 0.144601
 Thermal correction to Enthalpy= 0.145545
 Thermal correction to Gibbs Free Energy= 0.094969
 Sum of electronic and zero-point Energies= -693.804692
 Sum of electronic and thermal Energies= -693.792913
 Sum of electronic and thermal Enthalpies= -693.791968
 Sum of electronic and thermal Free Energies= -693.842544

[8-oxoG - H]⁻_1·W16

C1 0.915708 0.849364 -0.008201
 C2 0.573945 -0.481641 -0.013648
 C3 -0.798850 -0.869414 -0.004927
 C4 -1.213474 1.452662 -0.014546
 C5 2.861260 -0.376980 0.005152
 H6 2.869575 1.742174 0.000230
 H7 1.842491 -2.220797 -0.005895
 O8 -1.182969 -2.062563 0.009484
 O9 4.055596 -0.664131 0.011223
 N10 1.771993 -1.217610 -0.002641
 N11 2.308057 0.907609 0.004530
 N12 0.064593 1.882105 -0.005781
 N13 -1.677669 0.204784 -0.008529
 N14 -2.177566 2.467568 -0.068661
 H15 -3.076970 2.176437 0.285483
 H16 -1.849200 3.346600 0.304020
 O17 -4.003768 -1.680269 0.005708
 H18 -3.639107 -0.781554 -0.031929
 H19 -3.155052 -2.162298 0.021363
 Zero-point correction= 0.132610 (Hartree/Particle)
 Thermal correction to Energy= 0.144906
 Thermal correction to Enthalpy= 0.145850
 Thermal correction to Gibbs Free Energy= 0.093374
 Sum of electronic and zero-point Energies= -693.804055

Sum of electronic and thermal Energies= -693.791760
 Sum of electronic and thermal Enthalpies= -693.790816
 Sum of electronic and thermal Free Energies= -693.843291

[8-oxoG - H]⁻_1·W12

C1 -0.829605 -0.819362 -0.003756
 C2 -0.730888 0.549734 -0.049656
 C3 0.551242 1.181258 -0.111267
 C4 1.370672 -1.049230 -0.095913
 C5 -2.961308 0.042495 0.067899
 H6 -2.591614 -2.043597 0.104510
 H7 -2.289206 2.035950 -0.019356
 O8 0.728994 2.413271 -0.146549
 O9 -4.187545 0.114097 0.119735
 N10 -2.040621 1.061664 -0.004740
 N11 -2.188799 -1.122552 0.069783
 N12 0.187577 -1.690640 -0.026022
 N13 1.600176 0.267024 -0.122631
 N14 2.494467 -1.869385 -0.186120
 H15 3.367260 -1.414836 0.050199
 H16 2.360391 -2.787272 0.209459
 O17 4.272725 0.730326 0.359502
 H18 4.582159 1.481827 -0.153173
 H19 3.287340 0.714220 0.191130
 Zero-point correction= 0.132131 (Hartree/Particle)
 Thermal correction to Energy= 0.144518
 Thermal correction to Enthalpy= 0.145463
 Thermal correction to Gibbs Free Energy= 0.092855
 Sum of electronic and zero-point Energies= -693.803131
 Sum of electronic and thermal Energies= -693.790744
 Sum of electronic and thermal Enthalpies= -693.789799
 Sum of electronic and thermal Free Energies= -693.842407

[8-oxoG - H]⁻_1·W39

C1 -0.195214 0.372654 -0.042704
 C2 -0.500797 -0.961453 0.014790
 C3 0.540419 -1.947862 0.048635
 C4 1.984109 -0.083800 -0.031304
 C5 -2.479982 0.195259 -0.032468
 H6 -1.483950 2.080358 -0.107869
 H7 -2.432750 -1.909732 0.059818
 O8 0.330250 -3.172883 0.096423
 O9 -3.672844 0.489414 -0.039626
 N10 -1.904026 -1.055449 0.018499
 N11 -1.395035 1.076009 -0.073903
 N12 1.045257 0.891952 -0.066535
 N13 1.818735 -1.395469 0.013999
 N14 3.310598 0.376931 -0.007114
 H15 3.959064 -0.339316 -0.301642
 H16 3.437705 1.260590 -0.480510
 O17 0.654884 3.638739 0.061053
 H18 0.860933 3.868258 0.971561
 H19 0.940764 2.691074 -0.020462
 Zero-point correction= 0.132162 (Hartree/Particle)
 Thermal correction to Energy= 0.144563
 Thermal correction to Enthalpy= 0.145507
 Thermal correction to Gibbs Free Energy= 0.092544
 Sum of electronic and zero-point Energies= -693.799516
 Sum of electronic and thermal Energies= -693.787115

Sum of electronic and thermal Enthalpies= -693.786171
 Sum of electronic and thermal Free Energies= -693.839134

[8-oxoG - H]⁻_1-W23

C1 -0.195559 -0.472674 -0.127014
 C2 -0.876719 0.707555 0.014043
 C3 -0.170267 1.954077 0.101231
 C4 1.751826 0.611943 -0.152780
 C5 -2.436980 -0.969803 -0.034814
 H6 -0.966711 -2.474005 -0.289977
 H7 -2.995801 1.050768 0.165980
 O8 -0.733048 3.052871 0.255248
 O9 -3.489822 -1.603720 -0.036274
 N10 -2.245581 0.387269 0.074816
 N11 -1.143850 -1.493889 -0.146857
 N12 1.139003 -0.599426 -0.212537
 N13 1.208790 1.810133 -0.000279
 N14 3.139844 0.571939 -0.306662
 H15 3.597746 1.391443 0.062510
 H16 3.570182 -0.310405 -0.063974
 O17 2.827106 -2.754121 0.302923
 H18 2.671247 -2.880614 1.243150
 H19 2.168215 -2.056203 0.043771
 Zero-point correction= 0.132075 (Hartree/Particle)
 Thermal correction to Energy= 0.144502
 Thermal correction to Enthalpy= 0.145446
 Thermal correction to Gibbs Free Energy= 0.092556
 Sum of electronic and zero-point Energies= -693.799116
 Sum of electronic and thermal Energies= -693.786689
 Sum of electronic and thermal Enthalpies= -693.785745
 Sum of electronic and thermal Free Energies= -693.838635

[8-oxoG - H]⁻_1-W89

C1 -0.065436 -0.508108 -0.019781
 C2 -0.384770 0.827175 0.009269
 C3 -1.754159 1.252593 0.030248
 C4 -2.204881 -1.060283 0.013634
 C5 1.887035 0.679850 -0.045818
 H6 1.896952 -1.425368 -0.076158
 H7 0.917575 2.542719 0.001606
 O8 -2.103008 2.448799 0.042092
 O9 3.100953 0.957781 -0.065679
 N10 0.828276 1.540779 -0.008590
 N11 1.329917 -0.589572 -0.054021
 N12 -0.935699 -1.524352 -0.019923
 N13 -2.649128 0.191586 0.029026
 N14 -3.191106 -2.058950 0.069807
 H15 -4.086069 -1.728325 -0.261173
 H16 -2.892518 -2.931250 -0.342800
 O17 4.355746 -1.464996 0.002296
 H18 4.750305 -1.522597 0.876625
 H19 4.041660 -0.531651 -0.067185
 Zero-point correction= 0.132479 (Hartree/Particle)
 Thermal correction to Energy= 0.144734
 Thermal correction to Enthalpy= 0.145678
 Thermal correction to Gibbs Free Energy= 0.093346
 Sum of electronic and zero-point Energies= -693.796944
 Sum of electronic and thermal Energies= -693.784690
 Sum of electronic and thermal Enthalpies= -693.783745

Sum of electronic and thermal Free Energies= -693.836077

[8-oxoG - H]⁻_1-W8

C1 0.514582 -0.866933 -0.022449
 C2 0.163791 0.459101 -0.067455
 C3 1.172521 1.480083 -0.036300
 C4 2.660396 -0.347943 0.040778
 C5 -1.771973 -0.748046 -0.092118
 H6 -0.762906 -2.600567 -0.026343
 H7 -1.795821 1.352617 -0.168435
 O8 0.920224 2.698653 -0.051089
 O9 -2.963944 -1.094185 -0.120080
 N10 -1.243671 0.512926 -0.103994
 N11 -0.676885 -1.598225 -0.035942
 N12 1.758360 -1.355860 0.034407
 N13 2.461209 0.964226 0.019584
 N14 4.001737 -0.763659 0.040973
 H15 4.621571 -0.048574 0.393467
 H16 4.134369 -1.672486 0.461173
 O17 -5.108801 0.654341 0.130748
 H18 -5.139455 0.702702 1.090037
 H19 -4.378745 0.022410 -0.046465
 Zero-point correction= 0.131874 (Hartree/Particle)
 Thermal correction to Energy= 0.144618
 Thermal correction to Enthalpy= 0.145563
 Thermal correction to Gibbs Free Energy= 0.090549
 Sum of electronic and zero-point Energies= -693.796185
 Sum of electronic and thermal Energies= -693.783441
 Sum of electronic and thermal Enthalpies= -693.782496
 Sum of electronic and thermal Free Energies= -693.837510

[8-oxoG - H]⁻_2-W2

C1 0.792140 -0.784660 -0.009647
 C2 0.886195 0.597956 -0.008137
 C3 -0.283589 1.389283 -0.039592
 C4 -1.469685 -0.838846 -0.058423
 C5 3.027783 -0.206058 0.038923
 H6 -2.316031 1.042938 -0.108111
 H7 2.375907 -2.224712 0.025299
 H8 2.640814 1.858608 0.023105
 O9 -0.376789 2.624845 -0.046993
 O10 4.251271 -0.304295 0.064618
 N11 2.256357 0.929867 0.023070
 N12 2.102881 -1.256299 0.019880
 N13 -0.298045 -1.542051 -0.031792
 N14 -1.424298 0.565479 -0.063347
 N15 -2.661005 -1.381936 -0.078066
 H16 -2.558363 -2.392143 -0.082956
 O17 -4.935950 0.154243 0.052343
 H18 -5.044789 0.228648 1.004426
 H19 -4.154101 -0.463167 -0.048468
 Zero-point correction= 0.131646 (Hartree/Particle)
 Thermal correction to Energy= 0.144219
 Thermal correction to Enthalpy= 0.145163
 Thermal correction to Gibbs Free Energy= 0.090927
 Sum of electronic and zero-point Energies= -693.799271
 Sum of electronic and thermal Energies= -693.786697
 Sum of electronic and thermal Enthalpies= -693.785753
 Sum of electronic and thermal Free Energies= -693.839989

[8-oxoG - H]₂-W67

C1 -0.423707 -1.114363 0.007737
 C2 0.249923 0.107086 -0.021630
 C3 -0.491712 1.297532 -0.038748
 C4 -2.509298 -0.213262 0.016928
 C5 1.853416 -1.516311 -0.012427
 H6 -2.469710 1.847698 -0.027465
 H7 0.413961 -3.079986 0.032479
 H8 2.361093 0.543796 -0.042037
 O9 -0.072849 2.484529 -0.067876
 O10 2.915939 -2.130910 -0.007130
 N11 1.635131 -0.164694 -0.039384
 N12 0.569508 -2.086234 0.011846
 N13 -1.725264 -1.344567 0.027602
 N14 -1.861272 1.042007 -0.016278
 N15 -3.808181 -0.185352 0.034987
 H16 -4.136022 -1.148369 0.056982
 O17 2.612602 2.634577 -0.003412
 H18 2.823643 3.060160 0.831726
 H19 1.620323 2.678914 -0.066915
 Zero-point correction= 0.132635 (Hartree/Particle)
 Thermal correction to Energy= 0.144562
 Thermal correction to Enthalpy= 0.145507
 Thermal correction to Gibbs Free Energy= 0.094254
 Sum of electronic and zero-point Energies= -693.798128
 Sum of electronic and thermal Energies= -693.786201
 Sum of electronic and thermal Enthalpies= -693.785257
 Sum of electronic and thermal Free Energies= -693.836509

[8-oxoG - H]₂-W3

C1 -0.215798 0.344004 -0.035559
 C2 -0.287101 -1.037558 -0.003183
 C3 0.896493 -1.809399 0.029002
 C4 2.071116 0.437019 -0.031640
 C5 -2.438067 -0.252590 -0.017098
 H6 2.921747 -1.432888 0.022766
 H7 -1.782679 1.785347 -0.061191
 H8 -2.030572 -2.314372 0.022824
 O9 1.011093 -3.043597 0.068311
 O10 -3.662706 -0.174437 -0.016477
 N11 -1.654112 -1.382743 0.011883
 N12 -1.525571 0.807528 -0.046693
 N13 0.871662 1.115524 -0.049977
 N14 2.023679 -0.971311 0.010377
 N15 3.252975 0.975270 -0.046903
 H16 3.141676 1.985810 -0.086374
 O17 -0.277671 3.623386 0.009540
 H18 -0.064800 4.012921 0.862044
 H19 0.308615 2.821626 -0.050999
 Zero-point correction= 0.131985 (Hartree/Particle)
 Thermal correction to Energy= 0.144372
 Thermal correction to Enthalpy= 0.145317
 Thermal correction to Gibbs Free Energy= 0.092587
 Sum of electronic and zero-point Energies= -693.797017
 Sum of electronic and thermal Energies= -693.784629
 Sum of electronic and thermal Enthalpies= -693.783685
 Sum of electronic and thermal Free Energies= -693.836414

[8-oxoG - H]₂-W39

C1 0.215693 0.343819 -0.039304
 C2 0.287213 -1.037644 -0.004432
 C3 -0.896323 -1.809446 0.030663
 C4 -2.071124 0.436885 -0.033603
 C5 2.438251 -0.252222 -0.018098
 H6 -2.921610 -1.432994 0.025058
 H7 1.782391 1.785032 -0.064685
 H8 2.031058 -2.314069 0.025696
 O9 -1.010841 -3.043542 0.073308
 O10 3.662856 -0.173579 -0.015961
 N11 1.654432 -1.382539 0.012267
 N12 1.525247 0.807214 -0.051930
 N13 -0.871716 1.115401 -0.054140
 N14 -2.023573 -0.971413 0.010716
 N15 -3.253015 0.975099 -0.048731
 H16 -3.141780 1.985588 -0.090211
 O17 0.276966 3.623549 0.016581
 H18 0.065165 4.008480 0.871441
 H19 -0.308969 2.821872 -0.047359
 Zero-point correction= 0.131989 (Hartree/Particle)
 Thermal correction to Energy= 0.144375
 Thermal correction to Enthalpy= 0.145320
 Thermal correction to Gibbs Free Energy= 0.092593
 Sum of electronic and zero-point Energies= -693.797012
 Sum of electronic and thermal Energies= -693.784626
 Sum of electronic and thermal Enthalpies= -693.783681
 Sum of electronic and thermal Free Energies= -693.836408

[8-oxoG - H]₂-W6

C1 -1.057878 0.806584 0.024397
 C2 -0.479748 -0.457710 -0.054175
 C3 0.916569 -0.581821 -0.113791
 C4 0.910278 1.939944 -0.012805
 C5 -2.743662 -0.776178 0.033866
 H6 2.541306 0.686873 -0.147696
 H7 -3.136043 1.306089 0.136398
 H8 -1.423869 -2.402508 -0.108892
 O9 1.583705 -1.641408 -0.178523
 O10 -3.864840 -1.274710 0.057843
 N11 -1.525658 -1.404967 -0.039860
 N12 -2.433400 0.588236 0.077896
 N13 -0.465851 1.986574 0.050022
 N14 1.532247 0.670522 -0.090248
 N15 1.704999 2.965635 -0.005826
 H16 1.128282 3.802013 0.051685
 O17 4.309579 -1.942114 0.105393
 H18 4.355680 -1.902861 1.064473
 H19 3.347377 -1.850668 -0.082509
 Zero-point correction= 0.131366 (Hartree/Particle)
 Thermal correction to Energy= 0.144291
 Thermal correction to Enthalpy= 0.145236
 Thermal correction to Gibbs Free Energy= 0.089653
 Sum of electronic and zero-point Energies= -693.794846
 Sum of electronic and thermal Energies= -693.781921
 Sum of electronic and thermal Enthalpies= -693.780977
 Sum of electronic and thermal Free Energies= -693.836559

[8-oxoG - H]₂-W89

C1 0.071198 -0.520751 -0.036085
 C2 0.401803 0.828765 -0.010518
 C3 1.755284 1.229509 0.029912
 C4 2.215941 -1.261886 -0.003167
 C5 -1.869621 0.710950 -0.046173
 H6 3.581760 0.279722 0.052067
 H7 -1.902365 -1.396403 -0.084079
 H8 -0.892442 2.562181 -0.010491
 O9 2.216606 2.381956 0.063649
 O10 -3.078336 1.002272 -0.059556
 N11 -0.804923 1.560677 -0.013373
 N12 -1.326691 -0.566294 -0.059151
 N13 0.873983 -1.571276 -0.034656
 N14 2.587907 0.102381 0.027475
 N15 3.191965 -2.119633 0.002230
 H16 2.782206 -3.050833 -0.022371
 O17 -4.372470 -1.409672 0.015792
 H18 -4.050166 -0.480815 -0.053621
 H19 -4.748708 -1.470803 0.897928
 Zero-point correction= 0.132020 (Hartree/Particle)
 Thermal correction to Energy= 0.144468
 Thermal correction to Enthalpy= 0.145412
 Thermal correction to Gibbs Free Energy= 0.092263
 Sum of electronic and zero-point Energies= -693.793163
 Sum of electronic and thermal Energies= -693.780715
 Sum of electronic and thermal Enthalpies= -693.779771
 Sum of electronic and thermal Free Energies= -693.832919

[8-oxoG - H]₂-W8

C1 0.510783 -0.905055 -0.008062
 C2 0.075700 0.413431 -0.043674
 C3 1.019481 1.467061 -0.026204
 C4 2.724009 -0.410535 0.032854
 C5 -1.789160 -0.890390 -0.044153
 H6 3.071547 1.619173 0.016773
 H7 -0.681159 -2.689164 0.007523
 H8 -1.954796 1.190742 -0.113432
 O9 0.812845 2.689464 -0.036900
 O10 -2.964017 -1.295831 -0.055847
 N11 -1.336619 0.395317 -0.057925
 N12 -0.651099 -1.683520 -0.010328
 N13 1.744850 -1.379303 0.028714
 N14 2.320864 0.943705 0.006966
 N15 4.005099 -0.626871 0.060604
 H16 4.145971 -1.634621 0.077631
 O17 -4.537308 0.959426 0.024722
 H18 -4.097022 0.082310 -0.051660
 H19 -4.803247 1.014720 0.946587
 Zero-point correction= 0.131960 (Hartree/Particle)
 Thermal correction to Energy= 0.144468
 Thermal correction to Enthalpy= 0.145412
 Thermal correction to Gibbs Free Energy= 0.091687
 Sum of electronic and zero-point Energies= -693.792651
 Sum of electronic and thermal Energies= -693.780143
 Sum of electronic and thermal Enthalpies= -693.779198
 Sum of electronic and thermal Free Energies= -693.832923

**Cartesian coordinates for the structures in
Fig. 3a, optimized at B3LYP/6-311++G(d,p)**

[2,4-OO-8-oxoG + H]⁺

C1 -0.341722 -0.765913 -0.079484
 C2 -0.579813 0.717083 -0.049478
 C3 0.612601 1.554415 -0.030504
 C4 1.852435 -0.429978 -0.224893
 C5 -2.619787 -0.318132 -0.145489
 H6 -1.879202 -2.264486 -0.196779
 H7 -2.306099 1.861812 0.076669
 O8 0.382025 2.857615 0.084867
 O9 -3.798557 -0.377939 -0.145126
 N10 -1.848594 0.957235 -0.024241
 N11 -1.640520 -1.282942 -0.259152
 N12 0.734574 -1.021956 -0.959074
 N13 1.763738 1.010649 -0.125763
 N14 3.108282 -0.805663 -0.652214
 H15 3.846350 -0.179150 -0.359694
 H16 3.342907 -1.784119 -0.543222
 H17 1.215965 3.356135 0.079196
 H18 0.881690 -2.001150 -1.190175
 O19 0.151645 -0.998257 1.299797
 O20 1.581605 -0.923314 1.192485
 Zero-point correction= 0.139892 (Hartree/Particle)
 Thermal correction to Energy= 0.150872
 Thermal correction to Enthalpy= 0.151816
 Thermal correction to Gibbs Free Energy= 0.103993
 Sum of electronic and zero-point Energies= -768.507241
 Sum of electronic and thermal Energies= -768.496261
 Sum of electronic and thermal Enthalpies= -768.495317
 Sum of electronic and thermal Free Energies= -768.543139

[2,5-OO-8-oxoG + H]⁺

C1 -0.406167 -0.887443 -0.451605
 C2 -0.406162 0.414085 0.326906
 C3 0.555281 1.378369 -0.342757
 C4 1.875223 -0.411106 -0.095090
 C5 -2.584525 -0.316296 -0.036765
 H6 -1.983426 -2.152470 -1.032509
 H7 -2.160624 1.506846 0.915526
 O8 0.115474 2.594441 -0.588773
 O9 -3.762259 -0.428943 -0.052993
 N10 -1.774838 0.680066 0.479703
 N11 -1.649107 -1.284273 -0.628216
 N12 0.791501 -1.323699 -0.698477
 N13 1.720614 0.926165 -0.591087
 N14 3.132453 -0.947582 -0.328894
 H15 3.845302 -0.235235 -0.428149
 H16 3.405157 -1.686144 0.310140
 H17 0.824003 3.146077 -0.962700
 H18 1.043591 -2.198495 -1.148046
 O19 0.214668 0.040122 1.598862
 O20 1.592086 -0.430741 1.331703
 Zero-point correction= 0.140594 (Hartree/Particle)
 Thermal correction to Energy= 0.151409
 Thermal correction to Enthalpy= 0.152353
 Thermal correction to Gibbs Free Energy= 0.104963

Sum of electronic and zero-point Energies= -768.532984
 Sum of electronic and thermal Energies= -768.522169
 Sum of electronic and thermal Enthalpies= -768.521225
 Sum of electronic and thermal Free Energies= -768.568615

TS7⁺

C1 -0.356560 -0.754095 -0.144843
 C2 -0.559061 0.702443 -0.088235
 C3 0.625356 1.508683 -0.099077
 C4 1.885871 -0.431789 -0.357680
 C5 -2.610282 -0.285375 -0.170653
 H6 -1.880537 -2.250491 -0.246135
 H7 -2.304215 1.845293 0.125196
 O8 0.453873 2.817622 0.022563
 O9 -3.789536 -0.383226 -0.142571
 N10 -1.855101 0.951330 -0.045884
 N11 -1.630554 -1.273880 -0.329690
 N12 0.776141 -1.129841 -0.865422
 N13 1.786117 0.943592 -0.182223
 N14 3.116684 -0.885117 -0.631235
 H15 3.886236 -0.273740 -0.396856
 H16 3.309053 -1.876193 -0.624897
 H17 1.309262 3.277409 0.018654
 H18 0.905955 -2.118168 -1.054227
 O19 0.089500 -0.775348 1.398349
 O20 1.434823 -0.819785 1.436955
 Zero-point correction= 0.138638 (Hartree/Particle)
 Thermal correction to Energy= 0.149642
 Thermal correction to Enthalpy= 0.150586
 Thermal correction to Gibbs Free Energy= 0.102740
 Sum of electronic and zero-point Energies= -768.504353
 Sum of electronic and thermal Energies= -768.493349
 Sum of electronic and thermal Enthalpies= -768.492405
 Sum of electronic and thermal Free Energies= -768.540251

TS6⁺

C1 -0.419046 -0.805440 -0.412922
 C2 -0.494802 0.571832 0.022336
 C3 0.628798 1.409695 -0.308698
 C4 1.889793 -0.499378 -0.315319
 C5 -2.614058 -0.277687 -0.112999
 H6 -1.947527 -2.250696 -0.651347
 H7 -2.222215 1.728375 0.457204
 O8 0.426301 2.713158 -0.355160
 O9 -3.789400 -0.414305 -0.042908
 N10 -1.825357 0.854596 0.137105
 N11 -1.659311 -1.291125 -0.506120
 N12 0.782002 -1.308499 -0.683564
 N13 1.791490 0.858580 -0.452379
 N14 3.109668 -1.049872 -0.441627
 H15 3.885166 -0.411845 -0.321213
 H16 3.267041 -1.990044 -0.105919
 H17 1.265037 3.184811 -0.489177
 H18 0.922888 -2.294758 -0.873328
 O19 0.129471 -0.198545 1.620402
 O20 1.420635 -0.451024 1.574602
 Zero-point correction= 0.138712 (Hartree/Particle)
 Thermal correction to Energy= 0.149972
 Thermal correction to Enthalpy= 0.150916

Thermal correction to Gibbs Free Energy= 0.102571
 Sum of electronic and zero-point Energies= -768.507865
 Sum of electronic and thermal Energies= -768.496605
 Sum of electronic and thermal Enthalpies= -768.495660
 Sum of electronic and thermal Free Energies= -768.544006

[8-oxoG + H]⁺

C1 -0.296319 -0.796479 0.000002
 C2 -0.401439 0.584625 0.000012
 C3 0.782814 1.318509 0.000002
 C4 2.053560 -0.607050 0.000013
 C5 -2.520214 -0.272369 0.000002
 H6 -1.809383 -2.301206 -0.000012
 H7 -2.167042 1.809409 0.000018
 O8 0.726593 2.637952 -0.000016
 O9 -3.704614 -0.419935 -0.000002
 N10 -1.755367 0.887517 0.000011
 N11 -1.534369 -1.328467 -0.000002
 N12 0.922335 -1.403340 -0.000002
 N13 1.973898 0.708998 0.000033
 N14 3.253024 -1.206114 -0.000136
 H15 4.073913 -0.618998 0.000195
 H16 3.379884 -2.205329 0.000632
 H17 1.622397 3.011760 -0.000023
 H18 0.997343 -2.413348 -0.000175
 Zero-point correction= 0.132779 (Hartree/Particle)
 Thermal correction to Energy= 0.142861
 Thermal correction to Enthalpy= 0.143805
 Thermal correction to Gibbs Free Energy= 0.097751
 Sum of electronic and zero-point Energies= -618.211365
 Sum of electronic and thermal Energies= -618.201283
 Sum of electronic and thermal Enthalpies= -618.200339
 Sum of electronic and thermal Free Energies= -618.246393

TS1⁺

C1 -0.232248 -0.768965 -0.098865
 C2 -0.323145 0.693571 -0.185125
 C3 0.882761 1.411751 -0.103229
 C4 2.095422 -0.543884 -0.345588
 C5 -2.412653 -0.169817 -0.534575
 H6 -1.820213 -2.164844 -0.366673
 H7 -2.006609 1.938471 -0.399973
 O8 0.835371 2.728800 -0.038615
 O9 -3.590027 -0.207648 -0.691188
 N10 -1.608728 1.006426 -0.349837
 N11 -1.481804 -1.223552 -0.523499
 N12 0.972499 -1.295999 -0.584359
 N13 2.042798 0.769053 -0.091625
 N14 3.294582 -1.114870 -0.432901
 H15 4.109766 -0.528851 -0.317150
 H16 3.429141 -2.107640 -0.550990
 H17 1.732121 3.098449 0.012910
 H18 1.045566 -2.286823 -0.778052
 O19 -0.746246 -0.068682 2.149345
 O20 -0.134851 -1.036483 1.565429
 Zero-point correction= 0.137656 (Hartree/Particle)
 Thermal correction to Energy= 0.149462
 Thermal correction to Enthalpy= 0.150406
 Thermal correction to Gibbs Free Energy= 0.100251

Sum of electronic and zero-point Energies= -768.480675
 Sum of electronic and thermal Energies= -768.468869
 Sum of electronic and thermal Enthalpies= -768.467925
 Sum of electronic and thermal Free Energies= -768.518080

[4,5-dioxetane + H]⁺

C1 -0.289313 -0.839326 0.409719
 C2 -0.397314 0.671587 0.246025
 C3 0.890693 1.334641 -0.167685
 C4 2.011883 -0.674199 -0.338588
 C5 -2.310075 -0.297681 -0.619454
 H6 -1.911057 -2.202385 0.138675
 H7 -1.966465 1.780962 -0.689017
 O8 0.823023 2.632415 -0.268950
 O9 -3.425221 -0.397171 -1.021444
 N10 -1.530771 0.880058 -0.543125
 N11 -1.470119 -1.346264 -0.172453
 N12 0.932990 -1.432543 -0.076585
 N13 1.991653 0.690329 -0.379651
 N14 3.176123 -1.235003 -0.622188
 H15 3.949201 -0.630708 -0.867640
 H16 3.335518 -2.231789 -0.584378
 H17 1.688406 3.013495 -0.503976
 H18 0.973233 -2.438608 -0.185964
 O19 -0.536650 0.778687 1.702914
 O20 -0.261553 -0.683573 1.846255
 Zero-point correction= 0.141179 (Hartree/Particle)
 Thermal correction to Energy= 0.152428
 Thermal correction to Enthalpy= 0.153372
 Thermal correction to Gibbs Free Energy= 0.104231
 Sum of electronic and zero-point Energies= -768.543261
 Sum of electronic and thermal Energies= -768.532013
 Sum of electronic and thermal Enthalpies= -768.531069
 Sum of electronic and thermal Free Energies= -768.580209

TS2⁺

C1 -0.272158 -0.882723 0.268542
 C2 -0.383416 0.634987 0.135018
 C3 0.879459 1.361766 -0.206133
 C4 2.077614 -0.619237 -0.267371
 C5 -2.286437 -0.240405 -0.662699
 H6 -1.720039 -2.268073 -0.437945
 H7 -1.684962 0.967844 1.180217
 O8 0.773646 2.649477 -0.321373
 O9 -3.400894 -0.388605 -1.042608
 N10 -1.642582 0.971860 -0.286558
 N11 -1.336606 -1.333212 -0.507494
 N12 1.030138 -1.422150 0.000126
 N13 2.001775 0.739017 -0.383176
 N14 3.279810 -1.135515 -0.462552
 H15 4.035874 -0.505288 -0.696633
 H16 3.482500 -2.122126 -0.381907
 H17 1.629218 3.055144 -0.551740
 H18 1.148286 -2.428346 -0.008600
 O19 -0.638275 0.679670 1.723497
 O20 -0.523103 -0.811228 1.736741
 Zero-point correction= 0.134745 (Hartree/Particle)
 Thermal correction to Energy= 0.145753
 Thermal correction to Enthalpy= 0.146697

Thermal correction to Gibbs Free Energy= 0.098096
 Sum of electronic and zero-point Energies= -768.442575
 Sum of electronic and thermal Energies= -768.431567
 Sum of electronic and thermal Enthalpies= -768.430623
 Sum of electronic and thermal Free Energies= -768.479224

TS3⁺

C1 -0.293143 -0.834747 0.214281
 C2 -0.369965 0.682849 0.171048
 C3 0.955106 1.333513 -0.125621
 C4 2.031698 -0.702426 -0.305258
 C5 -2.275577 -0.319365 -0.666490
 H6 -1.540323 -1.157395 1.341955
 H7 -1.877051 1.772132 -0.859888
 O8 0.940414 2.631710 -0.180021
 O9 -3.388440 -0.357748 -1.075666
 N10 -1.438626 0.872988 -0.701618
 N11 -1.520067 -1.370522 -0.070982
 N12 0.907037 -1.445693 -0.125876
 N13 2.049369 0.656517 -0.300837
 N14 3.183014 -1.302980 -0.534204
 H15 3.996136 -0.726864 -0.713591
 H16 3.296400 -2.307801 -0.525008
 H17 1.828885 2.991703 -0.358363
 H18 0.890619 -2.447024 -0.296967
 O19 -0.650112 0.787078 1.620217
 O20 -0.545422 -0.680522 1.862811
 Zero-point correction= 0.135297 (Hartree/Particle)
 Thermal correction to Energy= 0.146188
 Thermal correction to Enthalpy= 0.147133
 Thermal correction to Gibbs Free Energy= 0.098854
 Sum of electronic and zero-point Energies= -768.453666
 Sum of electronic and thermal Energies= -768.442774
 Sum of electronic and thermal Enthalpies= -768.441830
 Sum of electronic and thermal Free Energies= -768.490109

TS4⁺

C1 -0.223761 -0.879757 -0.119569
 C2 -0.376484 0.484171 0.525737
 C3 0.686212 1.413078 -0.056672
 C4 2.017563 -0.406460 -0.490576
 C5 -2.361146 -0.181969 -0.517688
 H6 -1.508076 -2.002985 -1.336648
 H7 -2.230757 1.609381 0.569792
 O8 0.391070 2.684303 -0.044766
 O9 -3.477086 -0.238735 -0.914589
 N10 -1.736004 0.785264 0.257585
 N11 -1.318355 -1.157253 -0.811519
 N12 1.082048 -1.372959 -0.292308
 N13 1.784789 0.954169 -0.550294
 N14 3.273601 -0.776384 -0.637581
 H15 3.992210 -0.072920 -0.743797
 H16 3.525386 -1.755759 -0.661190
 H17 1.107189 3.213645 -0.440387
 H18 0.937500 -1.692681 0.925442
 O19 -0.003838 0.079348 1.840006
 O20 -0.145183 -1.387780 1.604125
 Zero-point correction= 0.136001 (Hartree/Particle)
 Thermal correction to Energy= 0.146861

Thermal correction to Enthalpy= 0.147805
 Thermal correction to Gibbs Free Energy= 0.099605
 Sum of electronic and zero-point Energies= -768.484726
 Sum of electronic and thermal Energies= -768.473867
 Sum of electronic and thermal Enthalpies= -768.472922
 Sum of electronic and thermal Free Energies= -768.521123

TS5⁺

C1 -0.293291 -0.301258 0.820946
 C2 -0.341521 0.618882 -0.369840
 C3 1.077779 1.125972 -0.655220
 C4 1.874220 -0.921307 -0.108265
 C5 -2.206720 -0.696074 -0.459287
 H6 -1.990957 -1.482922 1.482269
 H7 -1.599225 0.599732 -2.067807
 O8 1.195652 2.359359 -0.514591
 O9 -3.253326 -1.099063 -0.842182
 N10 -1.323154 0.195470 -1.181346
 N11 -1.533078 -0.980903 0.734010
 N12 0.879643 -1.126032 0.833301
 N13 2.021635 0.219198 -0.778341
 N14 2.772854 -1.884208 -0.288435
 H15 3.543775 -1.699108 -0.916226
 H16 2.787232 -2.739205 0.246796
 H17 0.162682 2.425972 0.319953
 H18 0.808076 -2.030794 1.279757
 O19 -0.734079 1.791389 0.732647
 O20 -0.220707 0.823860 1.755491
 Zero-point correction= 0.136012 (Hartree/Particle)
 Thermal correction to Energy= 0.146881
 Thermal correction to Enthalpy= 0.147825
 Thermal correction to Gibbs Free Energy= 0.099906
 Sum of electronic and zero-point Energies= -768.494099
 Sum of electronic and thermal Energies= -768.483230
 Sum of electronic and thermal Enthalpies= -768.482285
 Sum of electronic and thermal Free Energies= -768.530204

[4-OOH⁶-8-oxoG + H]⁺

C1 -0.236467 -0.748499 0.075972
 C2 -0.226910 0.768040 -0.042047
 C3 1.048564 1.541416 0.210643
 C4 2.118413 -0.443878 -0.421803
 C5 -2.268100 0.012164 -0.804028
 H6 -1.924694 -1.987099 -0.443927
 H7 -1.615164 2.142960 -0.653666
 O8 0.962721 2.694189 0.566681
 O9 -3.375398 0.147046 -1.189603
 N10 -1.352311 1.168427 -0.492114
 N11 -1.481525 -1.084092 -0.564341
 N12 0.960565 -1.210143 -0.551689
 N13 2.163544 0.822630 -0.060235
 N14 3.267289 -1.048415 -0.726737
 H15 4.110751 -0.492632 -0.684267
 H16 3.337816 -2.015452 -1.003310
 H17 -1.021453 -0.615001 3.005211
 H18 1.041238 -2.208293 -0.703661
 O19 -1.355370 -0.674059 2.094435
 O20 -0.162507 -1.184525 1.420615
 Zero-point correction= 0.138617 (Hartree/Particle)

Thermal correction to Energy= 0.151137
 Thermal correction to Enthalpy= 0.152082
 Thermal correction to Gibbs Free Energy= 0.099906
 Sum of electronic and zero-point Energies= -768.534003
 Sum of electronic and thermal Energies= -768.521483
 Sum of electronic and thermal Enthalpies= -768.520538
 Sum of electronic and thermal Free Energies= -768.572714

[4-OOH⁷-8-oxoG + H]⁺

C1 -0.316786 -0.758295 0.072039
 C2 -0.303673 0.762459 -0.076879
 C3 1.001247 1.407893 0.152854
 C4 2.048269 -0.563246 -0.424550
 C5 -2.262075 0.130069 -0.814250
 H6 -2.036048 -1.913571 -0.431711
 H7 -1.595402 -1.260729 2.716572
 O8 0.999893 2.660939 0.492470
 O9 -3.387720 0.226242 -1.172219
 N10 -1.358100 1.267128 -0.557495
 N11 -1.529739 -1.051877 -0.588538
 N12 0.906447 -1.273474 -0.528880
 N13 2.103244 0.738879 -0.020913
 N14 3.209919 -1.110413 -0.745654
 H15 4.038164 -0.531819 -0.697884
 H16 3.308974 -2.071870 -1.038736
 H17 1.909417 3.000035 0.575493
 H18 0.933830 -2.250687 -0.795262
 O19 -1.258846 -0.532228 2.170813
 O20 -0.213731 -1.209495 1.422261
 Zero-point correction= 0.139658 (Hartree/Particle)
 Thermal correction to Energy= 0.151844
 Thermal correction to Enthalpy= 0.152789
 Thermal correction to Gibbs Free Energy= 0.101499
 Sum of electronic and zero-point Energies= -768.541193
 Sum of electronic and thermal Energies= -768.529007
 Sum of electronic and thermal Enthalpies= -768.528062
 Sum of electronic and thermal Free Energies= -768.579352

[5-OOH⁹-8-oxoG + H]⁺

C1 -0.226915 -0.918496 -0.249148
 C2 -0.365138 0.535225 0.197691
 C3 0.847199 1.283258 -0.349020
 C4 2.117775 -0.629257 -0.224514
 C5 -2.295897 -0.416809 -0.658279
 H6 -1.528606 0.264434 2.846657
 H7 -2.188220 1.625450 -0.104283
 O8 0.659240 2.529233 -0.665837
 O9 -3.437731 -0.561515 -0.947580
 N10 -1.657448 0.787947 -0.298571
 N11 -1.279866 -1.470968 -0.668174
 N12 1.047136 -1.462792 -0.178716
 N13 2.001947 0.706207 -0.455698
 N14 3.341433 -1.111279 -0.108229
 H15 4.120025 -0.471616 -0.200862
 H16 3.535325 -2.082563 0.093477
 H17 1.479488 2.939689 -0.995786
 H18 1.148525 -2.468168 -0.280926
 O19 -0.158871 0.695148 1.609335
 O20 -0.962775 -0.297186 2.292464

Zero-point correction= 0.139947 (Hartree/Particle)
 Thermal correction to Energy= 0.151990
 Thermal correction to Enthalpy= 0.152934
 Thermal correction to Gibbs Free Energy= 0.102093
 Sum of electronic and zero-point Energies= -768.548313
 Sum of electronic and thermal Energies= -768.536270
 Sum of electronic and thermal Enthalpies= -768.535326
 Sum of electronic and thermal Free Energies= -768.586167

[5-OOH³-8-oxoG + H]⁺

C1 -0.295219 -1.001264 0.031153
 C2 -0.406441 0.524172 0.100686
 C3 0.782939 1.100627 -0.654274
 C4 1.901693 -0.862256 -0.328023
 C5 -2.492587 -0.422569 -0.246848
 H6 -1.803013 -2.452272 -0.017063
 H7 -2.171929 1.642385 -0.348439
 O8 0.628374 2.323042 -1.086806
 O9 -3.664148 -0.566659 -0.372671
 N10 -1.723452 0.735073 -0.377822
 N11 -1.540661 -1.473529 0.023223
 N12 0.822902 -1.647278 -0.048974
 N13 1.874417 0.434639 -0.797943
 N14 3.090054 -1.416041 -0.239240
 H15 3.915222 -0.886751 -0.488562
 H16 3.176935 -2.376836 0.066298
 H17 1.443009 2.645807 -1.512073
 H18 0.734457 0.784107 2.950829
 O19 -0.396049 0.989671 1.458506
 O20 0.944347 0.776603 2.003237
 Zero-point correction= 0.140613 (Hartree/Particle)
 Thermal correction to Energy= 0.152552
 Thermal correction to Enthalpy= 0.153496
 Thermal correction to Gibbs Free Energy= 0.102882
 Sum of electronic and zero-point Energies= -768.571033
 Sum of electronic and thermal Energies= -768.559093
 Sum of electronic and thermal Enthalpies= -768.558149
 Sum of electronic and thermal Free Energies= -768.608764

**Cartesian coordinates for the structures in Fig. 4,
optimized at B3LYP/6-311++G(d,p)**

[2,5-OO-8-oxoG + H]⁺·W

C1	0.356306	-1.199166	-0.433207
C2	-0.257264	-0.014796	0.308851
C3	0.179246	1.267738	-0.389081
C4	2.176527	-0.013211	-0.090155
C5	-1.859546	-1.657204	-0.066792
H6	-0.521054	-3.036643	-0.991140
H7	-2.284654	0.117815	0.993428
O8	-0.545499	2.271877	-0.713900
O9	-2.889515	-2.252664	-0.028669
N10	-1.609788	-0.352493	0.405452
N11	-0.634987	-2.098634	-0.627929
N12	1.607107	-1.205492	-0.668602
N13	1.463845	1.225832	-0.606885
N14	3.544444	0.087644	-0.295478
H15	4.035994	0.665207	0.377172
H16	3.980393	-0.816396	-0.429081
O17	0.434746	0.042012	1.594440
O18	1.896971	0.016682	1.345993
H19	-1.525141	2.234219	-0.445573
H20	1.987909	1.982450	-1.038716
O21	-3.003684	2.371951	0.064103
H22	-3.739853	2.182277	-0.532949
H23	-3.243708	3.174031	0.547531
Zero-point correction=	0.165028 (Hartree/Particle)		
Thermal correction to Energy=	0.178775		
Thermal correction to Enthalpy=	0.179719		
Thermal correction to Gibbs Free Energy=	0.125445		
Sum of electronic and zero-point Energies=	-844.994743		
Sum of electronic and thermal Energies=	-844.980996		
Sum of electronic and thermal Enthalpies=	-844.980051		
Sum of electronic and thermal Free Energies=	-845.034325		

TS6⁺·W

C1	0.276931	-1.254815	-0.336508
C2	-0.399963	0.000597	-0.028997
C3	0.267522	1.204032	-0.465500
C4	2.215545	-0.157287	-0.277898
C5	-1.958581	-1.670734	-0.084090
H6	-0.521664	-3.211492	-0.433993
H7	-2.472876	0.376501	0.260335
O8	-0.245575	2.375566	-0.674220
O9	-2.997850	-2.246102	-0.001414
N10	-1.732267	-0.278452	0.039007
N11	-0.679515	-2.215967	-0.345114
N12	1.559450	-1.350224	-0.432638
N13	1.581486	1.042756	-0.672189
N14	3.557311	-0.177806	-0.322404
H15	4.079112	0.612207	0.030058
H16	3.979992	-1.084188	-0.172783
O17	0.370351	0.417189	1.570614
O18	1.652133	0.074501	1.612039
H19	-1.216444	2.451042	-0.445081
H20	2.140654	1.872768	-0.845440

O21	-2.778736	2.536536	0.066442
H22	-2.945106	3.041447	0.874674
H23	-3.460227	2.807293	-0.564131
Zero-point correction=	0.163682 (Hartree/Particle)		
Thermal correction to Energy=	0.177791		
Thermal correction to Enthalpy=	0.178735		
Thermal correction to Gibbs Free Energy=	0.123690		
Sum of electronic and zero-point Energies=	-844.972310		
Sum of electronic and thermal Energies=	-844.958202		
Sum of electronic and thermal Enthalpies=	-844.957257		
Sum of electronic and thermal Free Energies=	-845.012302		

[8-oxoG + H]⁺·W + ¹O₂

C1	0.239744	-1.238147	-0.301163
C2	-0.463287	0.003274	-0.324544
N3	-0.691290	-2.207438	-0.172775
N4	1.547468	-1.386883	-0.389842
C5	0.281136	1.152069	-0.508088
N6	-1.803487	-0.276216	-0.227776
O7	-0.111063	2.397204	-0.613495
N8	1.638177	0.970768	-0.608208
C9	2.246632	-0.263834	-0.522946
N10	3.576058	-0.329179	-0.644473
C11	-2.002408	-1.659003	-0.095277
O12	-3.029202	-2.252042	0.043666
H13	-0.510671	-3.199834	-0.094068
H14	-2.552651	0.400075	-0.146756
H15	-1.083589	2.517366	-0.447838
H16	2.192420	1.816760	-0.689536
H17	4.170366	0.484804	-0.639435
H18	4.008247	-1.234910	-0.531673
O19	-2.737560	2.587425	-0.124991
H20	-3.314731	2.989773	-0.788111
H21	-3.000693	2.969523	0.723432
O22	0.355406	0.406150	1.976852
O23	1.573908	0.347879	2.146420
Zero-point correction=	0.163378 (Hartree/Particle)		
Thermal correction to Energy=	0.179303		
Thermal correction to Enthalpy=	0.180247		
Thermal correction to Gibbs Free Energy=	0.120294		
Sum of electronic and zero-point Energies=	-844.985177		
Sum of electronic and thermal Energies=	-844.969253		
Sum of electronic and thermal Enthalpies=	-844.968309		
Sum of electronic and thermal Free Energies=	-845.028261		

TS1⁺·W

C1	0.490946	-1.185545	-0.047437
C2	-0.387007	0.056735	0.192402
C3	0.286193	1.276786	-0.339646
C4	2.344851	0.003415	-0.354209
C5	-1.718179	-1.754567	-0.332212
H6	-0.101736	-3.157024	-0.431133
H7	-2.499725	0.156888	-0.036212
O8	-0.259489	2.413861	-0.596674
O9	-2.671750	-2.445951	-0.498123
N10	-1.659179	-0.353011	-0.279585
N11	-0.364684	-2.201238	-0.223477
N12	1.758016	-1.175728	-0.411072
N13	1.625857	1.214910	-0.390029

N14 3.668743 0.099551 -0.400220
 H15 4.170157 0.973364 -0.350696
 H16 4.200289 -0.759804 -0.358895
 H17 -1.255975 2.452613 -0.422867
 O18 -0.309194 0.328549 1.576100
 O19 0.849976 -0.408410 1.958372
 H20 2.120755 2.094592 -0.511777
 O21 -2.792634 2.494366 -0.037985
 H22 -3.434397 2.807321 -0.689873
 H23 -3.036725 2.900392 0.805220
 Zero-point correction= 0.163669 (Hartree/Particle)
 Thermal correction to Energy= 0.177573
 Thermal correction to Enthalpy= 0.178517
 Thermal correction to Gibbs Free Energy= 0.123755
 Sum of electronic and zero-point Energies= -844.957703
 Sum of electronic and thermal Energies= -844.943799
 Sum of electronic and thermal Enthalpies= -844.942855
 Sum of electronic and thermal Free Energies= -844.997617

Dioxetane [4,5-OO-8-oxoG + H]⁺·W

C1 0.547785 -1.030521 0.494924
 C2 -0.452937 0.097695 0.193434
 C3 0.202749 1.367743 -0.289661
 C4 2.346693 0.175352 -0.270628
 C5 -1.324688 -1.892474 -0.613922
 H6 0.279461 -3.102308 0.007549
 H7 -2.351740 -0.057397 -0.750285
 O8 -0.419921 2.465802 -0.485632
 O9 -2.115048 -2.648818 -1.091291
 N10 -1.433415 -0.464688 -0.629979
 N11 -0.121321 -2.175527 0.015890
 N12 1.903161 -0.946388 0.133858
 N13 1.509704 1.348688 -0.472468
 N14 3.646290 0.419848 -0.529793
 H15 3.951345 1.181001 -1.116461
 H16 4.282506 -0.357924 -0.421391
 H17 -1.420545 2.432258 -0.267870
 O18 -0.714101 0.250506 1.605228
 O19 0.363314 -0.733289 1.935989
 H20 1.949013 2.230482 -0.725661
 O21 -2.910427 2.289534 0.046102
 H22 -3.555539 2.780624 -0.480665
 H23 -3.213580 2.323079 0.964177
 Zero-point correction= 0.164802 (Hartree/Particle)
 Thermal correction to Energy= 0.179130
 Thermal correction to Enthalpy= 0.180074
 Thermal correction to Gibbs Free Energy= 0.123809
 Sum of electronic and zero-point Energies= -844.985270
 Sum of electronic and thermal Energies= -844.970942
 Sum of electronic and thermal Enthalpies= -844.969998
 Sum of electronic and thermal Free Energies= -845.026263

**Cartesian coordinates for the structures in Fig. 5,
optimized at B3LYP/6-311++G(d,p)**

Fig. 5a

[8-oxoG – H]⁻

C1	-0.202556	-0.777137	-0.008885
C2	-0.341296	0.588519	-0.012938
C3	0.813517	1.437744	-0.002628
C4	2.000600	-0.598367	-0.015307
C5	-2.453302	-0.300447	0.004804
H6	-1.730378	-2.290890	-0.004171
H7	-2.133645	1.780964	-0.004199
O8	0.754397	2.683011	0.012331
O9	-3.675900	-0.443746	0.010095
N10	-1.722015	0.863478	-0.001580
N11	-1.491677	-1.313892	-0.003799
N12	0.953667	-1.452932	-0.008865
N13	2.008972	0.728937	-0.003809
N14	3.262482	-1.218073	-0.071863
H15	3.992624	-0.615562	0.280584
H16	3.261641	-2.143135	0.334339
Zero-point correction=		0.107675	(Hartree/Particle)
Thermal correction to Energy=		0.116958	
Thermal correction to Enthalpy=		0.117902	
Thermal correction to Gibbs Free Energy=		0.073151	
Sum of electronic and zero-point Energies=		-617.345274	
Sum of electronic and thermal Energies=		-617.335991	
Sum of electronic and thermal Enthalpies=		-617.335047	
Sum of electronic and thermal Free Energies=		-617.379798	

precursor

C1	0.000940	-0.869482	-0.261922
C2	-0.177026	0.533397	-0.290927
C3	0.997952	1.390601	-0.387974
C4	2.192937	-0.602620	-0.088840
C5	-2.221157	-0.420315	-0.586994
H6	-1.482652	-2.390731	-0.304741
H7	-1.947365	1.656897	-0.479638
O8	0.922619	2.601334	-0.610222
O9	-3.410678	-0.588669	-0.770403
N10	-1.492992	0.768730	-0.626297
N11	-1.244920	-1.420416	-0.427214
N12	1.156177	-1.492965	-0.150712
N13	2.190037	0.716222	-0.196721
N14	3.433005	-1.202290	0.059765
H15	4.153699	-0.578159	0.388213
H16	3.410516	-2.121060	0.474707
O17	-0.440718	0.374770	1.802062
O18	-1.719376	0.319890	1.954769
Zero-point correction=		0.113349	(Hartree/Particle)
Thermal correction to Energy=		0.125404	
Thermal correction to Enthalpy=		0.126349	
Thermal correction to Gibbs Free Energy=		0.075378	
Sum of electronic and zero-point Energies=		-767.681118	
Sum of electronic and thermal Energies=		-767.669063	
Sum of electronic and thermal Enthalpies=		-767.668118	
Sum of electronic and thermal Free Energies=		-767.719089	

TS1⁻

C1	-0.007682	-0.883271	-0.225944
C2	-0.205235	0.540648	-0.146297
C3	0.991727	1.381383	-0.368441
C4	2.188248	-0.605932	-0.088486
C5	-2.222015	-0.415577	-0.556041
H6	-1.482153	-2.398890	-0.306150
H7	-1.973989	1.625956	-0.369003
O8	0.909605	2.576583	-0.637995
O9	-3.404422	-0.597913	-0.751291
N10	-1.495395	0.773846	-0.623861
N11	-1.242733	-1.424756	-0.395503
N12	1.148564	-1.499387	-0.148324
N13	2.186438	0.711883	-0.204806
N14	3.420375	-1.206038	0.056311
H15	4.159908	-0.589834	0.354717
H16	3.407911	-2.137910	0.439652
O17	-0.404587	0.504896	1.648997
O18	-1.688429	0.254975	1.915953
Zero-point correction=		0.113039	(Hartree/Particle)
Thermal correction to Energy=		0.124297	
Thermal correction to Enthalpy=		0.125242	
Thermal correction to Gibbs Free Energy=		0.076007	
Sum of electronic and zero-point Energies=		-767.680455	
Sum of electronic and thermal Energies=		-767.669197	
Sum of electronic and thermal Enthalpies=		-767.668252	
Sum of electronic and thermal Free Energies=		-767.717487	

[5-OO-8-oxoG - H]⁻

C1	-0.042734	-0.890098	-0.225059
C2	-0.248272	0.572625	0.109712
C3	0.974027	1.373220	-0.352906
C4	2.163588	-0.606933	-0.122936
C5	-2.240499	-0.367284	-0.537331
H6	-2.049215	1.610805	-0.158014
O7	0.878487	2.536858	-0.701335
O8	-3.418216	-0.564597	-0.730964
N9	-1.534164	0.822756	-0.527848
N10	-1.254519	-1.399690	-0.478707
N11	1.102629	-1.496544	-0.226669
N12	2.174817	0.699775	-0.262448
N13	3.365251	-1.232538	0.051874
H14	4.139940	-0.648816	0.322228
H15	3.339415	-2.188849	0.365576
O16	-0.315240	0.724560	1.516631
O17	-1.463609	-0.026950	2.024688
H18	-1.496263	-2.377607	-0.524245
Zero-point correction=		0.114068	(Hartree/Particle)
Thermal correction to Energy=		0.125522	
Thermal correction to Enthalpy=		0.126466	
Thermal correction to Gibbs Free Energy=		0.076657	
Sum of electronic and zero-point Energies=		-767.685338	
Sum of electronic and thermal Energies=		-767.673884	
Sum of electronic and thermal Enthalpies=		-767.672940	
Sum of electronic and thermal Free Energies=		-767.722749	

TS2⁻

C1	-0.050996	-0.866123	-0.270215
C2	-0.237445	0.573238	0.096845

C3 1.003415 1.412295 -0.183692
 C4 2.163765 -0.599306 -0.181165
 C5 -2.202031 -0.304168 -0.640046
 H6 -1.948181 1.728551 -0.423299
 O7 0.920954 2.615198 -0.373867
 O8 -3.368152 -0.422125 -0.923253
 N9 -1.456904 0.865159 -0.608694
 N10 -1.311952 -1.429393 -0.327476
 N11 1.090426 -1.473978 -0.298269
 N12 2.189956 0.717929 -0.178105
 N13 3.361441 -1.246891 -0.122323
 H14 4.170156 -0.703746 0.130280
 H15 3.344748 -2.237910 0.051651
 O16 -0.409927 0.526368 1.536203
 O17 -1.542529 -0.295500 1.925063
 H18 -1.540512 -1.503810 0.741903
 Zero-point correction= 0.111346 (Hartree/Particle)
 Thermal correction to Energy= 0.122089
 Thermal correction to Enthalpy= 0.123034
 Thermal correction to Gibbs Free Energy= 0.075053
 Sum of electronic and zero-point Energies= -767.672972
 Sum of electronic and thermal Energies= -767.662229
 Sum of electronic and thermal Enthalpies= -767.661284
 Sum of electronic and thermal Free Energies= -767.709265

TS3⁻

C1 0.016459 -0.987696 0.017260
 C2 -0.274265 0.486029 0.003287
 C3 0.881280 1.215930 -0.689925
 C4 2.202370 -0.561107 0.012870
 C5 -2.193994 -0.683441 -0.458347
 H6 -1.308874 -2.616056 -0.158184
 O7 0.726459 2.225061 -1.347826
 O8 -3.341886 -1.004434 -0.661612
 N9 -1.612492 0.575010 -0.523889
 N10 -1.166124 -1.617822 -0.136505
 N11 1.192247 -1.520082 0.112316
 N12 2.131596 0.670730 -0.422601
 N13 3.433868 -1.061284 0.327955
 H14 4.171861 -0.388328 0.457133
 H15 3.458306 -1.921389 0.850579
 O16 -0.256724 0.982425 1.397924
 O17 -1.611064 1.243072 1.846015
 H18 -2.100340 1.212622 0.162666
 Zero-point correction= 0.112177 (Hartree/Particle)
 Thermal correction to Energy= 0.123176
 Thermal correction to Enthalpy= 0.124120
 Thermal correction to Gibbs Free Energy= 0.075265
 Sum of electronic and zero-point Energies= -767.681619
 Sum of electronic and thermal Energies= -767.670620
 Sum of electronic and thermal Enthalpies= -767.669676
 Sum of electronic and thermal Free Energies= -767.718530

TS4⁻

C1 -0.112068 -0.853138 -0.269041
 C2 -0.259488 0.577042 0.256328
 C3 0.914806 1.417673 -0.297765
 C4 2.098970 -0.569524 -0.254652
 C5 -2.301434 -0.257321 -0.510353

H6 -1.571862 -2.221543 -0.911889
 H7 -2.112479 1.619981 0.255317
 O8 0.787401 2.589515 -0.601410
 O9 -3.489991 -0.416672 -0.694281
 N10 -1.607762 0.894213 -0.232564
 N11 -1.323418 -1.271684 -0.685606
 N12 1.026706 -1.437493 -0.436666
 N13 2.118338 0.743047 -0.319803
 N14 3.291831 -1.216788 -0.131493
 H15 4.075681 -0.662924 0.173161
 H16 3.256876 -2.193740 0.109847
 O17 -0.135009 0.592715 1.625897
 O18 -0.941499 -0.566713 2.103467
 Zero-point correction= 0.113876 (Hartree/Particle)
 Thermal correction to Energy= 0.124659
 Thermal correction to Enthalpy= 0.125603
 Thermal correction to Gibbs Free Energy= 0.077543
 Sum of electronic and zero-point Energies= -767.685093
 Sum of electronic and thermal Energies= -767.674310
 Sum of electronic and thermal Enthalpies= -767.673366
 Sum of electronic and thermal Free Energies= -767.721426

[5-OOH⁷-8-oxoG - H]⁻

C1 -0.027458 -1.084181 0.146301
 C2 -0.365731 0.393143 -0.002161
 C3 0.761225 1.087876 -0.800889
 C4 2.150743 -0.606600 -0.015682
 C5 -2.263331 -0.732908 -0.305689
 H6 -1.323489 -2.711651 0.092945
 O7 0.566101 2.037572 -1.529900
 O8 -3.394784 -1.160121 -0.480890
 N9 -1.712682 0.471924 -0.430712
 N10 -1.194224 -1.711018 0.104306
 N11 1.176168 -1.568680 0.230575
 N12 2.032123 0.581996 -0.551593
 N13 3.413771 -1.055402 0.260643
 H14 4.142348 -0.360710 0.280571
 H15 3.491253 -1.866024 0.852460
 O16 -0.243048 0.902751 1.391671
 O17 -0.945362 2.171847 1.431319
 H18 -1.712158 1.946271 0.852615
 Zero-point correction= 0.113796 (Hartree/Particle)
 Thermal correction to Energy= 0.125229
 Thermal correction to Enthalpy= 0.126173
 Thermal correction to Gibbs Free Energy= 0.076478
 Sum of electronic and zero-point Energies= -767.702452
 Sum of electronic and thermal Energies= -767.691018
 Sum of electronic and thermal Enthalpies= -767.690074
 Sum of electronic and thermal Free Energies= -767.739769

[4,5-dioxetane - H]⁻

C1 -0.170822 -0.839991 0.463439
 C2 -0.356405 0.675618 0.388717
 C3 0.804217 1.465392 -0.233088
 C4 1.924813 -0.587188 -0.386547
 C5 -2.182419 -0.361942 -0.623915
 H6 -1.380387 -2.263519 -0.547568
 H7 -1.873086 1.705229 -0.708940
 O8 0.635539 2.672827 -0.432302

O9 -3.172967 -0.513496 -1.317135
 N10 -1.622387 0.848260 -0.240706
 N11 -1.396758 -1.371843 -0.076297
 N12 0.991430 -1.440006 -0.002519
 N13 1.915605 0.768273 -0.526109
 N14 3.123036 -1.155583 -0.793821
 H15 3.894088 -0.506522 -0.817483
 H16 3.308022 -2.070687 -0.412801
 O17 -0.381638 0.756695 1.836675
 O18 -0.223612 -0.730969 1.951676
 Zero-point correction= 0.115431 (Hartree/Particle)
 Thermal correction to Energy= 0.126165
 Thermal correction to Enthalpy= 0.127109
 Thermal correction to Gibbs Free Energy= 0.078817
 Sum of electronic and zero-point Energies= -767.704681
 Sum of electronic and thermal Energies= -767.693947
 Sum of electronic and thermal Enthalpies= -767.693003
 Sum of electronic and thermal Free Energies= -767.741295

[5-OOH⁹-8-oxoG - H]⁻

C1 -0.153834 -0.916068 -0.308771
 C2 -0.301727 0.543348 0.137208
 C3 0.897402 1.392962 -0.371397
 C4 2.075398 -0.597279 -0.246883
 C5 -2.250474 -0.408966 -0.620761
 H6 -2.135784 1.617551 -0.042919
 O7 0.729852 2.571086 -0.654168
 O8 -3.438842 -0.513650 -0.856493
 N9 -1.610260 0.806255 -0.325727
 N10 -1.297405 -1.448258 -0.655992
 N11 1.051637 -1.485132 -0.278195
 N12 2.082602 0.732936 -0.406089
 N13 3.311418 -1.172740 -0.140485
 H14 4.094145 -0.565368 0.031758
 H15 3.355107 -2.147299 0.104135
 O16 -0.132568 0.669025 1.576261
 O17 -1.046550 -0.220555 2.282124
 H18 -0.575146 -1.067530 2.234279
 Zero-point correction= 0.113477 (Hartree/Particle)
 Thermal correction to Energy= 0.125348
 Thermal correction to Enthalpy= 0.126292
 Thermal correction to Gibbs Free Energy= 0.075652
 Sum of electronic and zero-point Energies= -767.720516
 Sum of electronic and thermal Energies= -767.708645
 Sum of electronic and thermal Enthalpies= -767.707701
 Sum of electronic and thermal Free Energies= -767.758341

Fig. 5b

[8-oxoG - H]⁻·W

C1 -0.393207 -1.110208 0.012926
 C2 0.247982 0.109354 -0.008625
 C3 -0.525830 1.307982 -0.029070
 C4 -2.376030 -0.131334 0.025780
 C5 1.872952 -1.496938 -0.013418
 H6 0.457780 -3.078968 0.032774
 H7 2.347808 0.576830 -0.032503
 O8 -0.029741 2.470298 -0.067621
 O9 2.945991 -2.096159 -0.012294

N10 1.632661 -0.145591 -0.030461
 N11 0.599032 -2.083610 0.006160
 N12 -1.716271 -1.306928 0.029484
 N13 -1.887425 1.104588 -0.008186
 N14 -3.774531 -0.233897 0.099212
 H15 -4.236025 0.590652 -0.257266
 H16 -4.126731 -1.101240 -0.279971
 O17 2.609384 2.613341 -0.019021
 H18 1.605569 2.636514 -0.075661
 H19 2.817060 3.061290 0.805093
 Zero-point correction= 0.132821 (Hartree/Particle)
 Thermal correction to Energy= 0.144601
 Thermal correction to Enthalpy= 0.145545
 Thermal correction to Gibbs Free Energy= 0.094969
 Sum of electronic and zero-point Energies= -693.804692
 Sum of electronic and thermal Energies= -693.792913
 Sum of electronic and thermal Enthalpies= -693.791968
 Sum of electronic and thermal Free Energies= -693.842544

precursor·W

C1 0.473505 -1.032086 -0.406634
 C2 -0.138159 0.221872 -0.200944
 C3 0.702667 1.397779 -0.103763
 C4 2.479018 -0.116006 -0.223833
 C5 -1.795615 -1.277396 -0.606903
 H6 -0.452939 -2.923606 -0.678314
 H7 -2.181099 0.797418 -0.272962
 O8 0.247458 2.561102 -0.049726
 O9 -2.877821 -1.791441 -0.815448
 N10 -1.489130 0.060983 -0.399190
 N11 -0.542248 -1.921870 -0.643547
 N12 1.775852 -1.259975 -0.428695
 N13 2.046071 1.132348 -0.075009
 N14 3.854618 -0.282934 -0.218851
 H15 4.357724 0.475686 0.215064
 H16 4.164303 -1.214398 0.012162
 O17 -0.116008 -0.471109 1.917643
 O18 -1.290745 -0.941088 2.071314
 O19 -2.427336 2.825689 -0.195559
 H20 -1.440180 2.829528 -0.077573
 H21 -2.576828 3.305307 -1.014673
 Zero-point correction= 0.138393 (Hartree/Particle)
 Thermal correction to Energy= 0.153190
 Thermal correction to Enthalpy= 0.154134
 Thermal correction to Gibbs Free Energy= 0.096863
 Sum of electronic and zero-point Energies= -844.135505
 Sum of electronic and thermal Energies= -844.120708
 Sum of electronic and thermal Enthalpies= -844.119764
 Sum of electronic and thermal Free Energies= -844.177035

TS1⁻·W

C1 0.520386 -1.067963 -0.334812
 C2 -0.158067 0.163048 0.019978
 C3 0.668180 1.390036 -0.107267
 C4 2.488563 -0.058110 -0.203588
 C5 -1.739938 -1.355264 -0.545964
 H6 -0.340707 -2.972929 -0.614408
 H7 -2.207037 0.640053 -0.134081
 O8 0.160755 2.519474 -0.162516

O9 -2.788243 -1.920360 -0.766080
 N10 -1.474501 0.001614 -0.429917
 N11 -0.455066 -1.973389 -0.562239
 N12 1.823780 -1.235935 -0.384296
 N13 2.015796 1.182080 -0.107100
 N14 3.855824 -0.183006 -0.181884
 H15 4.358336 0.611202 0.180888
 H16 4.214059 -1.103019 0.017827
 O17 -0.185208 -0.173562 1.709549
 O18 -1.204190 -1.018653 1.970107
 O19 -2.576386 2.841067 -0.193605
 H20 -1.595916 2.813948 -0.102364
 H21 -2.718129 3.056988 -1.119545
 Zero-point correction= 0.137698 (Hartree/Particle)
 Thermal correction to Energy= 0.151946
 Thermal correction to Enthalpy= 0.152890
 Thermal correction to Gibbs Free Energy= 0.096673
 Sum of electronic and zero-point Energies= -844.131925
 Sum of electronic and thermal Energies= -844.117678
 Sum of electronic and thermal Enthalpies= -844.116733
 Sum of electronic and thermal Free Energies= -844.172950

[5-OO-8-oxoG - H]·W

C1 0.391922 -0.971657 -0.539811
 C2 -0.155515 0.058932 0.426769
 C3 0.688326 1.333121 0.316654
 C4 2.410674 -0.052495 -0.370066
 C5 -1.880082 -1.153006 -0.488489
 H6 -2.180469 0.366146 0.794321
 O7 0.204643 2.443640 0.494888
 O8 -2.964309 -1.643569 -0.691159
 N9 -1.563568 0.099364 0.034944
 N10 -0.649678 -1.701684 -0.956157
 N11 1.643617 -1.106101 -0.845697
 N12 2.022078 1.122694 0.081487
 N13 3.747791 -0.264435 -0.498385
 H14 4.364677 0.385810 -0.040423
 H15 4.056765 -1.203524 -0.685786
 O16 0.001688 -0.415891 1.750541
 O17 -0.777970 -1.645567 1.901252
 H18 -0.604512 -2.592247 -1.427870
 O19 -2.315534 3.178173 -0.733834
 H20 -1.481414 3.116063 -0.236961
 H21 -2.476826 2.255230 -0.960462
 Zero-point correction= 0.138501 (Hartree/Particle)
 Thermal correction to Energy= 0.153261
 Thermal correction to Enthalpy= 0.154206
 Thermal correction to Gibbs Free Energy= 0.095913
 Sum of electronic and zero-point Energies= -844.135680
 Sum of electronic and thermal Energies= -844.120919
 Sum of electronic and thermal Enthalpies= -844.119975
 Sum of electronic and thermal Free Energies= -844.178268

TS2·W

C1 0.525197 -1.064144 -0.355411
 C2 -0.183152 0.139406 0.176747
 C3 0.626006 1.414096 -0.006781
 C4 2.465120 0.027244 -0.258789

C5 -1.697133 -1.349668 -0.621186
 H6 -2.234025 0.620190 -0.209766
 O7 0.080827 2.518780 -0.034630
 O8 -2.733011 -1.892888 -0.911101
 N9 -1.464791 0.002601 -0.452920
 N10 -0.416873 -2.062576 -0.457281
 N11 1.815081 -1.173621 -0.457820
 N12 1.973088 1.249487 -0.109942
 N13 3.819657 -0.085929 -0.281730
 H14 4.362173 0.713191 0.000232
 H15 4.213980 -1.010691 -0.241625
 O16 -0.215907 -0.139463 1.611919
 O17 -0.926784 -1.358890 1.914173
 H18 -0.528619 -2.352494 0.590583
 O19 -2.682233 2.826194 -0.128505
 H20 -1.710045 2.803771 0.004685
 H21 -2.785968 3.084831 -1.048589
 Zero-point correction= 0.135967 (Hartree/Particle)
 Thermal correction to Energy= 0.149864
 Thermal correction to Enthalpy= 0.150808
 Thermal correction to Gibbs Free Energy= 0.095345
 Sum of electronic and zero-point Energies= -844.122901
 Sum of electronic and thermal Energies= -844.109005
 Sum of electronic and thermal Enthalpies= -844.108061
 Sum of electronic and thermal Free Energies= -844.163523

TS3·W

C1 0.477122 -1.041625 -0.455440
 C2 -0.128723 0.051590 0.385274
 C3 0.657805 1.344558 0.134619
 C4 2.457085 -0.035841 -0.339368
 C5 -1.792805 -1.246082 -0.539981
 H6 -0.453871 -2.663837 -1.422549
 O7 0.137833 2.448367 0.150661
 O8 -2.854124 -1.748052 -0.816989
 N9 -1.547420 -0.020703 0.088192
 N10 -0.537456 -1.826275 -0.865829
 N11 1.734915 -1.158737 -0.737529
 N12 2.014657 1.158627 -0.020486
 N13 3.802900 -0.218995 -0.405774
 H14 4.386597 0.492533 0.001982
 H15 4.145215 -1.161111 -0.492601
 O16 0.089039 -0.244681 1.801212
 O17 -1.061042 -0.951791 2.332110
 H18 -1.982981 -0.087662 1.044186
 O19 -2.564388 2.825317 -0.888819
 H20 -1.680179 2.939250 -0.503506
 H21 -2.689413 1.874524 -0.773551
 Zero-point correction= 0.137025 (Hartree/Particle)
 Thermal correction to Energy= 0.151194
 Thermal correction to Enthalpy= 0.152138
 Thermal correction to Gibbs Free Energy= 0.095505
 Sum of electronic and zero-point Energies= -844.133428
 Sum of electronic and thermal Energies= -844.119259
 Sum of electronic and thermal Enthalpies= -844.118315
 Sum of electronic and thermal Free Energies= -844.174948

TS4·W

C1 0.451331 -0.968939 -0.502829

C2 -0.142320 0.046425 0.476489
 C3 0.528005 1.411662 0.200753
 C4 2.366149 0.163600 -0.421577
 C5 -1.802064 -1.308234 -0.446211
 H6 -0.455775 -2.570803 -1.512163
 H7 -2.193423 0.103226 0.949513
 O8 -0.079149 2.470269 0.283011
 O9 -2.846376 -1.895466 -0.617031
 N10 -1.576929 -0.090764 0.170038
 N11 -0.557448 -1.711220 -0.995365
 N12 1.687632 -0.963657 -0.872557
 N13 1.872020 1.328710 -0.054433
 N14 3.714591 0.051614 -0.518681
 H15 4.271638 0.771534 -0.088995
 H16 4.099375 -0.867862 -0.657579
 O17 0.183146 -0.293959 1.769430
 O18 -0.094538 -1.753446 1.868071
 O19 -2.819802 2.890198 -0.515986
 H20 -1.909320 2.885497 -0.170175
 H21 -2.944403 1.967785 -0.763345
 Zero-point correction= 0.138371 (Hartree/Particle)
 Thermal correction to Energy= 0.152418
 Thermal correction to Enthalpy= 0.153362
 Thermal correction to Gibbs Free Energy= 0.097052
 Sum of electronic and zero-point Energies= -844.135454
 Sum of electronic and thermal Energies= -844.121407
 Sum of electronic and thermal Enthalpies= -844.120463
 Sum of electronic and thermal Free Energies= -844.176773

[5-OOH⁷-8-oxoG - H]⁻·W

C1 -0.650038 1.222580 -0.060864
 C2 0.180422 -0.020920 0.229318
 C3 -0.495480 -1.241190 -0.438811
 C4 -2.479271 -0.044165 -0.268434
 C5 1.613882 1.631057 -0.221704
 H6 0.018452 3.157135 -0.439893
 O7 0.133095 -2.197212 -0.854839
 O8 2.549727 2.386712 -0.420609
 N9 1.528850 0.308859 -0.059915
 N10 0.229682 2.208063 -0.169779
 N11 -1.940425 1.236432 -0.210857
 N12 -1.876435 -1.194632 -0.456258
 N13 -3.841071 -0.045596 -0.223763
 H14 -4.299900 -0.935338 -0.121115
 H15 -4.303562 0.798592 0.068442
 O16 -0.013234 -0.196394 1.688873
 O17 0.961804 -1.169762 2.134373
 H18 1.765602 -0.829526 1.687023
 O19 3.117802 -2.016034 -0.935619
 H20 2.239875 -2.420647 -0.986946
 H21 2.864690 -1.104757 -0.697987
 Zero-point correction= 0.138805 (Hartree/Particle)
 Thermal correction to Energy= 0.153311
 Thermal correction to Enthalpy= 0.154255
 Thermal correction to Gibbs Free Energy= 0.097051
 Sum of electronic and zero-point Energies= -844.158786
 Sum of electronic and thermal Energies= -844.144280
 Sum of electronic and thermal Enthalpies= -844.143336
 Sum of electronic and thermal Free Energies= -844.200540

[4,5-dioxetane - H]⁻·W

C1 0.650621 -1.050993 0.360591
 C2 -0.331531 0.116947 0.479897
 C3 0.211069 1.477881 0.022577
 C4 2.210819 0.370161 -0.483303
 C5 -1.397628 -1.655086 -0.589483
 H6 0.310499 -2.808796 -0.773737
 H7 -2.342399 0.219735 -0.305082
 O8 -0.549640 2.465812 0.064073
 O9 -2.224629 -2.289706 -1.219383
 N10 -1.512931 -0.347959 -0.155283
 N11 -0.139334 -2.115416 -0.195596
 N12 1.905616 -0.881493 -0.216834
 N13 1.477011 1.523012 -0.393910
 N14 3.472464 0.591743 -1.007893
 H15 3.782147 1.549018 -0.948896
 H16 4.151411 -0.125991 -0.807442
 O17 -0.311148 -0.008520 1.931323
 O18 0.700153 -1.112864 1.847652
 O19 -3.206870 2.113242 -0.246854
 H20 -2.267217 2.347127 -0.039702
 H21 -3.377257 2.532527 -1.094697
 Zero-point correction= 0.140382 (Hartree/Particle)
 Thermal correction to Energy= 0.153926
 Thermal correction to Enthalpy= 0.154871
 Thermal correction to Gibbs Free Energy= 0.100041
 Sum of electronic and zero-point Energies= -844.158288
 Sum of electronic and thermal Energies= -844.144744
 Sum of electronic and thermal Enthalpies= -844.143799
 Sum of electronic and thermal Free Energies= -844.198629

[5-OOH⁹-8-oxoG - H]⁻·W

C1 0.516724 -1.110107 -0.389087
 C2 -0.213636 0.074728 0.254977
 C3 0.444480 1.404371 -0.207368
 C4 2.378611 0.147494 -0.344006
 C5 -1.611735 -1.524627 -0.623582
 H6 -2.347701 0.314759 0.169549
 O7 -0.247995 2.415192 -0.359591
 O8 -2.641829 -2.099313 -0.914515
 N9 -1.541516 -0.229610 -0.107278
 N10 -0.299315 -2.033843 -0.807875
 N11 1.855372 -1.088749 -0.444892
 N12 1.777837 1.354952 -0.375088
 N13 3.745305 0.193015 -0.271734
 H14 4.168684 1.085838 -0.467108
 H15 4.235179 -0.645254 -0.540557
 O16 0.033643 0.132597 1.684895
 O17 -0.275754 -1.146875 2.305598
 H18 0.556412 -1.629010 2.176335
 O19 -3.009101 2.514096 -0.018343
 H20 -2.030187 2.560936 -0.088086
 H21 -3.304549 2.465658 -0.932026
 Zero-point correction= 0.138622 (Hartree/Particle)
 Thermal correction to Energy= 0.153349
 Thermal correction to Enthalpy= 0.154293
 Thermal correction to Gibbs Free Energy= 0.096371

Sum of electronic and zero-point Energies=	-844.172115
Sum of electronic and thermal Energies=	-844.157388
Sum of electronic and thermal Enthalpies=	-844.156444
Sum of electronic and thermal Free Energies=	-844.214366