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Supporting Information

Capturing Transient Endoperoxide in the Singlet Oxygen Oxidation of Guanine

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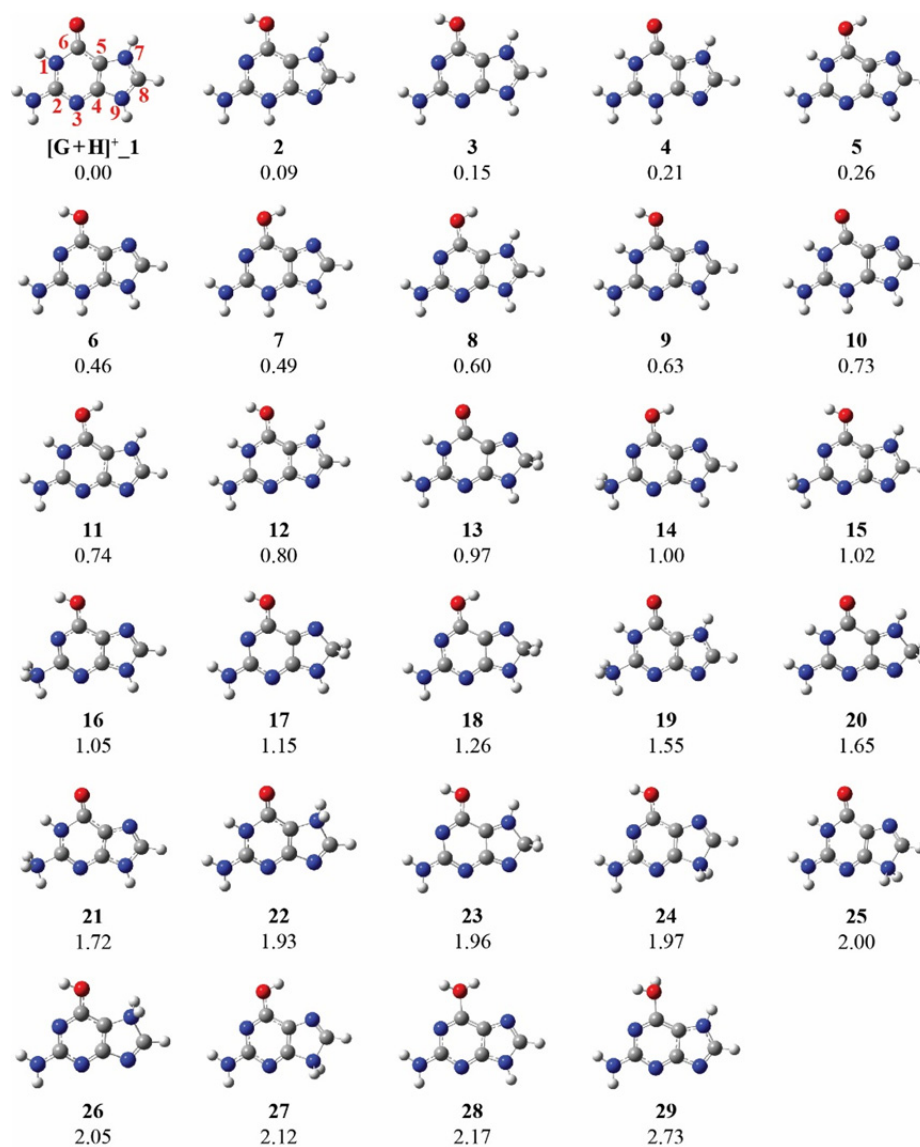


Fig. S1 Stable tautomers of $[G + H]^+$. Relative energies (eV, including thermal corrections at 298 K)

were calculated at B3LYP/6-311++G**.

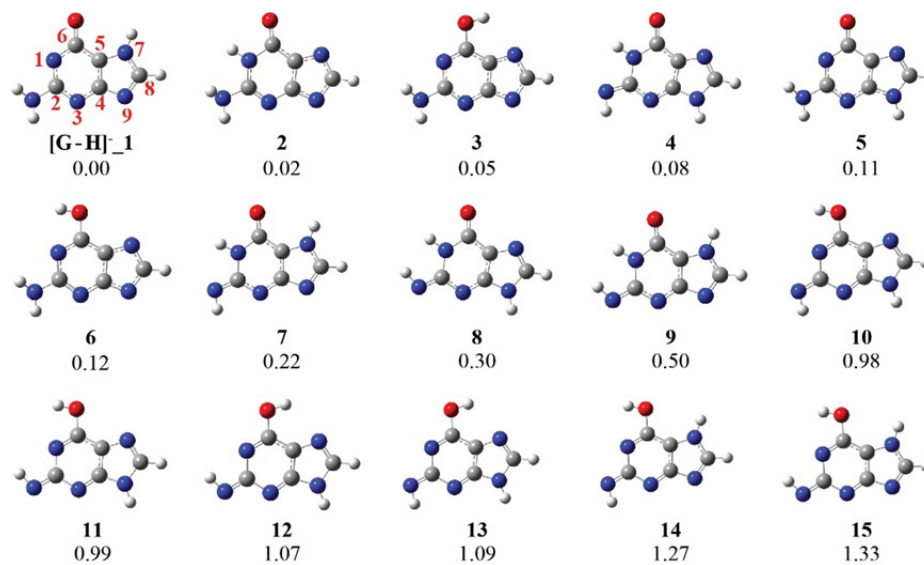


Fig. S2 Stable tautomers of $[G-H]^-$. Relative energies (eV, including thermal corrections at 298 K)

were calculated at B3LYP/6-311++G**.

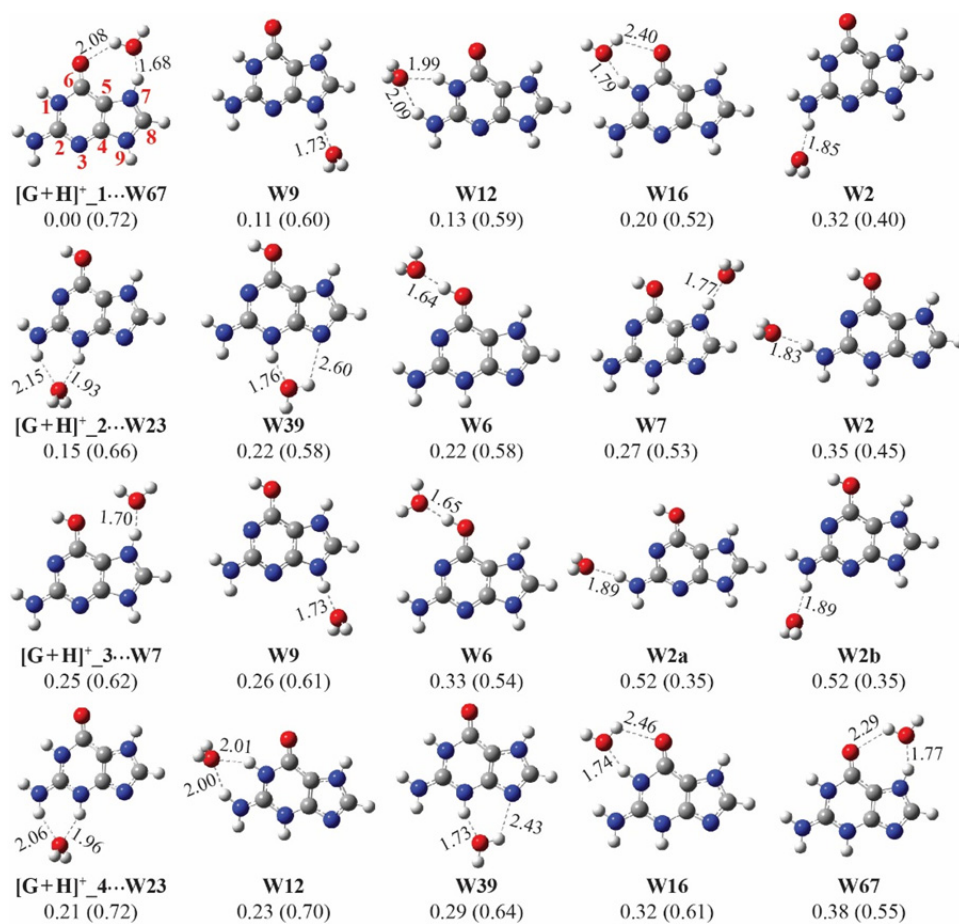


Fig. S3 Stable tautomers of $[G + H]^+(H_2O)$. Dashed lines indicate hydrogen bonds. Bond distances are shown in Å. Relative energies (eV, including thermal corrections at 298 K) and hydration energies (presented in parentheses) were calculated at B3LYP/6-311++G**.

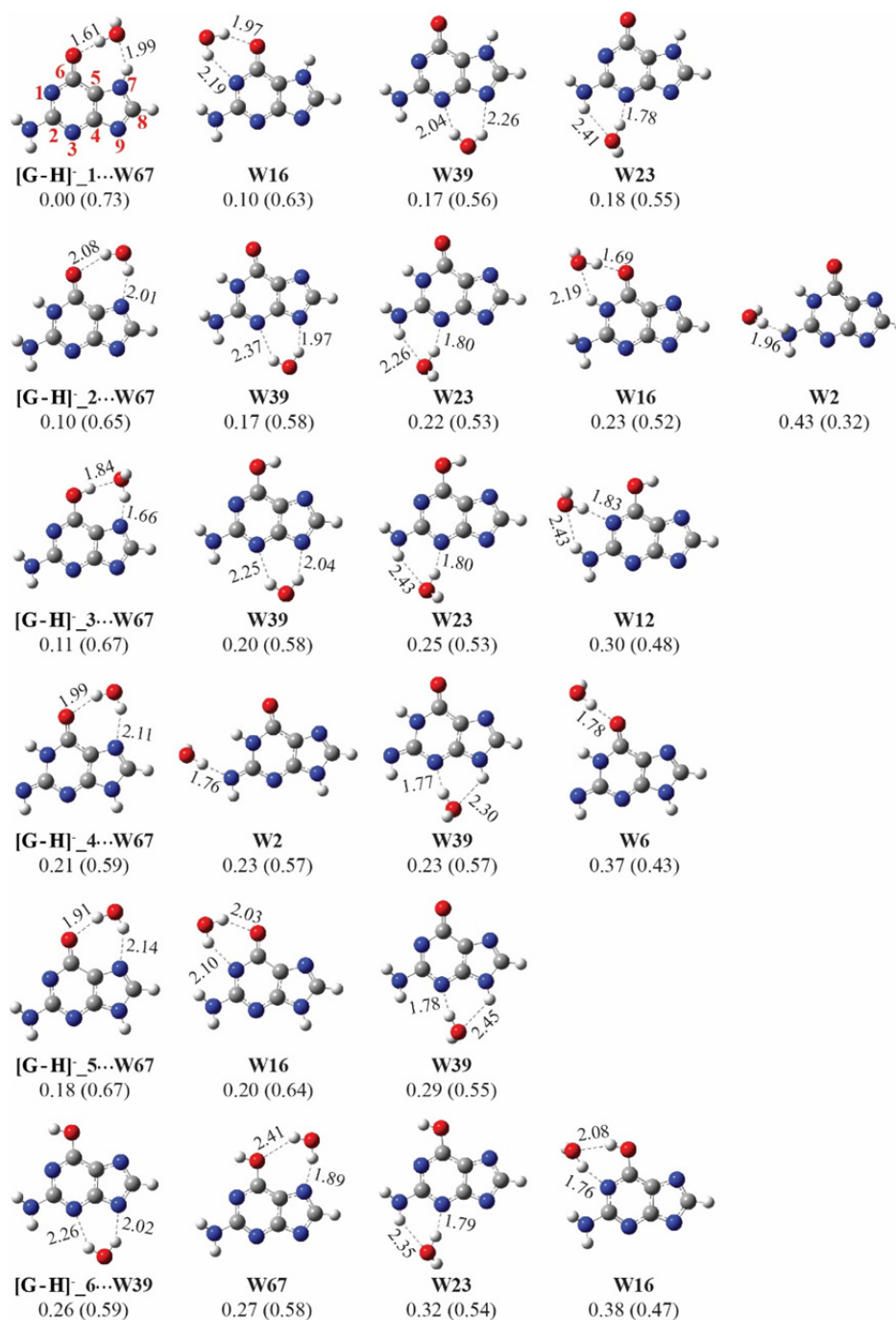


Fig. S4 Stable tautomers of $[G-H](H_2O)$. Dashed lines indicate hydrogen bonds. Bond distances are shown in Å. Relative energies (eV, including thermal corrections at 298 K) and hydration energies (presented in parentheses) were calculated at B3LYP/6-311++G**.

Cartesian coordinates for the structures of neutral guanine tautomers in Fig.1, optimized at B3LYP/6-311++G**

7H-keto

C1 -0.182583 1.446620 0.003320
 C2 0.819466 0.433780 0.011153
 H3 -2.235973 1.475286 -0.088773
 C4 -1.690703 -0.530967 -0.001773
 C5 2.643315 -0.778559 -0.001562
 N6 -1.460403 0.830781 -0.003587
 N7 2.195551 0.509312 0.008707
 N8 1.671057 -1.667682 -0.006203
 N9 -0.751047 -1.430457 0.008642
 C10 0.517061 -0.926612 -0.000327
 N11 -3.013354 -0.917480 -0.068236
 H12 -3.137075 -1.910153 0.072607
 H13 -3.693317 -0.346531 0.412410
 O14 -0.063538 2.663060 -0.005419
 H15 3.697110 -1.014676 -0.004925
 H16 2.745612 1.354712 0.011900

Zero-point correction= 0.116385 (Hartree/Particle)
 Thermal correction to Energy= 0.124677
 Thermal correction to Enthalpy= 0.125621
 Thermal correction to Gibbs Free Energy= 0.083293
 Sum of electronic and zero-point Energies= -542.597261
 Sum of electronic and thermal Energies= -542.588969
 Sum of electronic and thermal Enthalpies= -542.588025
 Sum of electronic and thermal Free Energies= -542.630353

9H-keto

C1 -0.208132 1.471732 0.002904
 C2 0.855107 0.503069 0.007608
 H3 -2.269156 1.417421 -0.072430
 C4 -1.674176 -0.564008 -0.002241
 H5 1.852101 -2.507064 -0.010624
 C6 2.713885 -0.532471 0.000457
 N7 -1.476726 0.791654 -0.002566
 N8 2.224474 0.676574 0.007123
 N9 1.729120 -1.506040 -0.003697
 N10 -0.696812 -1.433981 0.007702
 C11 0.527295 -0.850766 -0.000197
 N12 -2.975129 -1.004832 -0.064418
 H13 -3.077009 -1.996231 0.095417
 H14 -3.693025 -0.433735 0.355223
 O15 -0.186773 2.684777 -0.003287
 H16 3.762903 -0.787575 -0.001480

Zero-point correction= 0.116262 (Hartree/Particle)
 Thermal correction to Energy= 0.124556
 Thermal correction to Enthalpy= 0.125501
 Thermal correction to Gibbs Free Energy= 0.083193
 Sum of electronic and zero-point Energies= -542.596683
 Sum of electronic and thermal Energies= -542.588389
 Sum of electronic and thermal Enthalpies= -542.587445
 Sum of electronic and thermal Free Energies= -542.629752

9H-cis-enol

C1 -0.322205 1.307706 -0.000453
 C2 0.812236 0.485463 -0.003970
 C3 -1.663824 -0.568678 -0.004791
 C4 2.704782 -0.479992 0.001351
 N5 -1.538071 0.779685 -0.000306
 N6 2.179579 0.712085 -0.002770
 N7 1.760126 -1.496223 0.004212
 N8 -0.671452 -1.466519 0.002990
 C9 0.528910 -0.890048 0.000126
 N10 -2.944342 -1.049156 -0.052681
 H11 -3.076822 -2.023576 0.162837
 H12 -3.686552 -0.408277 0.173663
 O13 -0.209760 2.641719 0.005347
 H14 3.762888 -0.696491 0.002385
 H15 -1.109731 2.999109 0.001342
 H16 1.928024 -2.490329 0.003308

Zero-point correction= 0.116239 (Hartree/Particle)
 Thermal correction to Energy= 0.124483
 Thermal correction to Enthalpy= 0.125427
 Thermal correction to Gibbs Free Energy= 0.083337
 Sum of electronic and zero-point Energies= -542.594687
 Sum of electronic and thermal Energies= -542.586444
 Sum of electronic and thermal Enthalpies= -542.585500
 Sum of electronic and thermal Free Energies= -542.627589

9H-trans-enol

C1 -0.289466 1.318397 -0.001026
 C2 0.798798 0.434215 -0.005563
 C3 -1.704126 -0.488147 -0.004258
 C4 2.660727 -0.587186 0.001266
 N5 -1.523316 0.854606 -0.000032
 N6 2.170780 0.623014 -0.003870
 N7 1.682827 -1.569569 0.004603
 N8 -0.757380 -1.440967 0.003469
 C9 0.467846 -0.924054 -0.000137
 N10 -3.003922 -0.906539 -0.048515
 H11 -3.190489 -1.874296 0.154612
 H12 -3.716262 -0.224248 0.150990
 O13 -0.128984 2.652207 0.006132
 H14 3.711078 -0.837347 0.002804
 H15 0.819506 2.843247 0.006177
 H16 1.822440 -2.568187 0.005089

Zero-point correction= 0.116279 (Hartree/Particle)
 Thermal correction to Energy= 0.124559
 Thermal correction to Enthalpy= 0.125504
 Thermal correction to Gibbs Free Energy= 0.083339
 Sum of electronic and zero-point Energies= -542.593635
 Sum of electronic and thermal Energies= -542.585354
 Sum of electronic and thermal Enthalpies= -542.584410
 Sum of electronic and thermal Free Energies= -542.626575

7H-cis-enol

C1 -0.297452 1.295058 -0.000653
 C2 0.788922 0.428163 -0.007284
 C3 -1.683896 -0.536497 -0.004890

C4 2.641556 -0.745720 0.003212
N5 -1.525304 0.815734 0.000362
N6 2.168205 0.538403 -0.004258
N7 1.701844 -1.661180 0.006717
N8 -0.722355 -1.457072 0.003736
C9 0.517555 -0.952850 -0.000181
N10 -2.981362 -0.976914 -0.056948
H11 -3.133058 -1.948331 0.161736
H12 -3.701818 -0.320792 0.195066
O13 -0.109769 2.631445 0.006953
H14 3.702313 -0.951988 0.005185
H15 2.710807 1.387188 -0.010228
H16 -0.987407 3.040634 0.004139

Zero-point correction= 0.115958 (Hartree/Particle)
Thermal correction to Energy= 0.124298
Thermal correction to Enthalpy= 0.125242
Thermal correction to Gibbs Free Energy= 0.082967
Sum of electronic and zero-point Energies= -542.590275
Sum of electronic and thermal Energies= -542.581935
Sum of electronic and thermal Enthalpies= -542.580991
Sum of electronic and thermal Free Energies= -542.623266

Cartesian coordinates for the structures of protonated guanine tautomers in Fig. S1, optimized at B3LYP/6-311++G**

[G + H]⁺_1

C1 0.250467 1.473032 0.000018
 C2 -0.787307 0.475596 0.000028
 H3 2.304031 1.455404 -0.000255
 C4 1.726416 -0.543403 0.000013
 H5 -1.803224 -2.546384 -0.000033
 C6 -2.692643 -0.641734 -0.000014
 N7 1.514494 0.818303 0.000018
 N8 -2.166340 0.578342 0.000006
 N9 -1.690088 -1.539387 -0.000009
 N10 0.737351 -1.428423 0.000057
 C11 -0.471308 -0.870021 0.000013
 N12 2.992135 -0.984417 -0.000299
 H13 3.148083 -1.981055 0.000485
 H14 3.790936 -0.371321 0.001170
 O15 0.141159 2.675096 -0.000012
 H16 -3.744736 -0.875510 -0.000032
 H17 -2.690972 1.446359 0.000004

Zero-point correction= 0.129499 (Hartree/Particle)
 Thermal correction to Energy= 0.138080
 Thermal correction to Enthalpy= 0.139025
 Thermal correction to Gibbs Free Energy= 0.096132
 Sum of electronic and zero-point Energies= -542.960078
 Sum of electronic and thermal Energies= -542.951497
 Sum of electronic and thermal Enthalpies= -542.950553
 Sum of electronic and thermal Free Energies= -542.993446

[G + H]⁺_2

C1 -0.269828 1.323583 0.000004
 C2 0.820050 0.441424 -0.000004
 C3 -1.739818 -0.463279 0.000006
 C4 2.663724 -0.747538 -0.000005
 N5 -1.510283 0.851638 0.000013
 N6 2.199200 0.528790 -0.000010
 N7 1.696042 -1.657247 0.000006
 N8 -0.724934 -1.378241 0.000014
 C9 0.568772 -0.925952 0.000007
 N10 -3.007045 -0.891785 -0.000079
 H11 -3.261828 -1.866755 0.000186
 H12 -3.742711 -0.201174 0.000137
 O13 -0.061423 2.625955 0.000005
 H14 3.719056 -0.976966 -0.000010
 H15 2.754229 1.374123 -0.000023
 H16 -0.909432 3.099667 0.000002
 H17 -0.896195 -2.378047 0.000016

Zero-point correction= 0.129358 (Hartree/Particle)
 Thermal correction to Energy= 0.137874
 Thermal correction to Enthalpy= 0.138818
 Thermal correction to Gibbs Free Energy= 0.096156
 Sum of electronic and zero-point Energies= -542.956882
 Sum of electronic and thermal Energies= -542.948366
 Sum of electronic and thermal Enthalpies= -542.947422
 Sum of electronic and thermal Free Energies= -542.990084

[G + H]⁺_3

C1 -0.370326 1.320732 0.000004
 C2 0.749843 0.466386 -0.000017
 C3 -1.715699 -0.560013 0.000003
 C4 2.688145 -0.600255 -0.000006
 N5 -1.570616 0.798046 0.000021
 N6 2.131882 0.607508 -0.000027
 N7 1.718974 -1.529997 0.000020
 N8 -0.711841 -1.465065 0.000039
 C9 0.474016 -0.900116 0.000011
 N10 -2.971694 -1.022284 -0.000216
 H11 -3.141378 -2.015379 0.000499
 H12 -3.745418 -0.377492 0.000526
 O13 -0.182604 2.635382 0.000020
 H14 3.747363 -0.801090 -0.000012
 H15 -1.043491 3.084287 0.000017
 H16 1.866340 -2.532388 0.000028
 H17 2.644609 1.481133 -0.000050

Zero-point correction= 0.129698 (Hartree/Particle)
 Thermal correction to Energy= 0.138035
 Thermal correction to Enthalpy= 0.138980
 Thermal correction to Gibbs Free Energy= 0.096675
 Sum of electronic and zero-point Energies= -542.954352
 Sum of electronic and thermal Energies= -542.946015
 Sum of electronic and thermal Enthalpies= -542.945070
 Sum of electronic and thermal Free Energies= -542.987375

[G + H]⁺_4

C1 0.135121 1.481172 0.000019
 C2 -0.865520 0.460043 0.000021
 H3 2.215617 1.533945 -0.000097
 C4 1.756423 -0.457637 0.000020
 C5 -2.669792 -0.789339 -0.000030
 N6 1.459953 0.856567 0.000071
 N7 -2.242661 0.498738 -0.000022
 N8 -1.666831 -1.661050 0.000004
 N9 0.744506 -1.342132 0.000072
 C10 -0.569282 -0.887273 0.000030
 N11 3.026257 -0.874673 -0.000296
 H12 3.261306 -1.856014 0.000549
 H13 3.794485 -0.220822 0.000661
 O14 0.047373 2.677964 -0.000018
 H15 -3.715954 -1.055166 -0.000061
 H16 -2.817293 1.331865 -0.000043
 H17 0.912591 -2.341469 -0.000038

Zero-point correction= 0.128900 (Hartree/Particle)
 Thermal correction to Energy= 0.137736
 Thermal correction to Enthalpy= 0.138680
 Thermal correction to Gibbs Free Energy= 0.095304
 Sum of electronic and zero-point Energies= -542.952523
 Sum of electronic and thermal Energies= -542.943687
 Sum of electronic and thermal Enthalpies= -542.942742
 Sum of electronic and thermal Free Energies= -542.986119

[G + H]⁺_5

C1 0.203060 1.334860 -0.000002

C2 -0.843276 0.441558 -0.000003
 H3 2.233997 1.457722 0.000003
 C4 1.700038 -0.568494 0.000005
 H5 -1.843807 -2.570057 0.000000
 C6 -2.689636 -0.584807 -0.000005
 N7 1.461119 0.799721 0.000002
 N8 -2.210261 0.625018 -0.000006
 N9 -1.702214 -1.567982 -0.000002
 N10 0.721045 -1.454878 0.000004
 C11 -0.502037 -0.930608 0.000000
 N12 2.977270 -0.976855 0.000009
 H13 3.153042 -1.970663 0.000011
 H14 3.765835 -0.350501 0.000009
 O15 0.156765 2.647899 -0.000004
 H16 -3.738624 -0.842780 -0.000008
 H17 -0.762186 2.962868 -0.000006

Zero-point correction= 0.128957 (Hartree/Particle)
 Thermal correction to Energy= 0.137616
 Thermal correction to Enthalpy= 0.138560
 Thermal correction to Gibbs Free Energy= 0.095618
 Sum of electronic and zero-point Energies= -542.950434
 Sum of electronic and thermal Energies= -542.941775
 Sum of electronic and thermal Enthalpies= -542.940830
 Sum of electronic and thermal Free Energies= -542.983773

[G + H]⁺₆

C1 -0.291819 1.330783 0.000003
 C2 0.835177 0.478951 0.000007
 C3 -1.730666 -0.483126 0.000008
 C4 2.732554 -0.473366 0.000001
 N5 -1.527091 0.826515 0.000021
 N6 2.193807 0.706874 0.000007
 N7 1.781614 -1.502680 -0.000001
 N8 -0.693769 -1.389252 0.000001
 C9 0.577473 -0.885988 0.000002
 N10 -2.986527 -0.947034 -0.000091
 H11 -3.221553 -1.926676 0.000393
 H12 -3.737726 -0.272849 0.000155
 O13 -0.131440 2.629630 -0.000010
 H14 3.789467 -0.694403 -0.000003
 H15 -0.995955 3.072596 -0.000017
 H16 1.978420 -2.494508 -0.000007
 H17 -0.873689 -2.385686 -0.000116

Zero-point correction= 0.128659 (Hartree/Particle)
 Thermal correction to Energy= 0.137356
 Thermal correction to Enthalpy= 0.138300
 Thermal correction to Gibbs Free Energy= 0.095297
 Sum of electronic and zero-point Energies= -542.943122
 Sum of electronic and thermal Energies= -542.934425
 Sum of electronic and thermal Enthalpies= -542.933481
 Sum of electronic and thermal Free Energies= -542.976484

[G + H]⁺₇

C1 -0.265869 1.338759 0.000001
 C2 0.822314 0.436772 0.000003
 C3 -1.757900 -0.417986 0.000002
 C4 2.699292 -0.554267 0.000001

N5 -1.513193 0.883125 0.000006
 N6 2.184031 0.639348 0.000003
 N7 1.725154 -1.558263 -0.000001
 N8 -0.756350 -1.371385 -0.000001
 C9 0.531272 -0.916240 0.000000
 N10 -3.029599 -0.834308 -0.000027
 H11 -3.304857 -1.803419 0.000127
 H12 -3.750836 -0.127272 0.000044
 O13 -0.111959 2.641560 -0.000004
 H14 3.750952 -0.798372 -0.000001
 H15 0.830080 2.878413 -0.000004
 H16 1.901844 -2.554017 -0.000003
 H17 -0.976466 -2.359665 -0.000038

Zero-point correction= 0.128815 (Hartree/Particle)
 Thermal correction to Energy= 0.137482
 Thermal correction to Enthalpy= 0.138426
 Thermal correction to Gibbs Free Energy= 0.095480
 Sum of electronic and zero-point Energies= -542.942302
 Sum of electronic and thermal Energies= -542.933635
 Sum of electronic and thermal Enthalpies= -542.932691
 Sum of electronic and thermal Free Energies= -542.975637

[G + H]⁺₈

C1 0.373223 1.336160 -0.000005
 C2 -0.750246 0.470045 -0.000048
 C3 1.723411 -0.544712 -0.000007
 C4 -2.676828 -0.643297 -0.000006
 N5 1.566663 0.804925 -0.000007
 N6 -2.143879 0.576742 0.000014
 N7 -1.692496 -1.550731 0.000023
 N8 0.725114 -1.459727 0.000033
 C9 -0.458162 -0.899065 0.000000
 N10 2.982376 -0.996412 -0.000061
 H11 3.163864 -1.987395 0.000101
 H12 3.747414 -0.340520 0.000103
 O13 0.322734 2.670528 0.000041
 H14 -3.732633 -0.861855 -0.000039
 H15 -0.574298 3.023005 0.000049
 H16 -1.817303 -2.556446 0.000079
 H17 -2.701746 1.420627 -0.000242

Zero-point correction= 0.128697 (Hartree/Particle)
 Thermal correction to Energy= 0.137430
 Thermal correction to Enthalpy= 0.138374
 Thermal correction to Gibbs Free Energy= 0.095209
 Sum of electronic and zero-point Energies= -542.938098
 Sum of electronic and thermal Energies= -542.929365
 Sum of electronic and thermal Enthalpies= -542.928421
 Sum of electronic and thermal Free Energies= -542.971586

[G + H]⁺₉

C1 -0.215725 1.341141 0.000000
 C2 0.847790 0.464069 0.000002
 H3 -2.277595 1.383026 -0.000064
 C4 -1.682316 -0.605124 0.000004
 H5 1.874554 -2.544299 -0.000004
 C6 2.704093 -0.547572 0.000003
 N7 -1.469084 0.772244 -0.000001

N8 2.214228 0.655410 0.000007
 N9 1.726580 -1.543257 -0.000004
 N10 -0.688911 -1.466810 0.000005
 C11 0.524876 -0.916807 -0.000004
 N12 -2.954222 -1.035951 -0.000023
 H13 -3.109987 -2.033177 0.000025
 H14 -3.756646 -0.427989 0.000142
 O15 -0.060114 2.646133 -0.000013
 H16 3.755687 -0.795212 0.000004
 H17 -0.877540 3.162889 0.000092

Zero-point correction= 0.127449 (Hartree/Particle)
 Thermal correction to Energy= 0.136830
 Thermal correction to Enthalpy= 0.137774
 Thermal correction to Gibbs Free Energy= 0.092571
 Sum of electronic and zero-point Energies= -542.937720
 Sum of electronic and thermal Energies= -542.928339
 Sum of electronic and thermal Enthalpies= -542.927395
 Sum of electronic and thermal Free Energies= -542.972598

[G + H]⁺_10

C1 0.154335 1.499788 -0.000002
 C2 -0.890326 0.505204 -0.000003
 H3 2.248838 1.493079 0.000005
 C4 1.751227 -0.479790 0.000005
 H5 -1.908142 -2.511339 0.000000
 C6 -2.746669 -0.532014 -0.000006
 N7 1.480579 0.829432 0.000002
 N8 -2.252902 0.671175 -0.000007
 N9 -1.755847 -1.511711 -0.000002
 N10 0.713518 -1.348203 0.000004
 C11 -0.577189 -0.838160 0.000000
 N12 3.007887 -0.937472 0.000012
 H13 3.219519 -1.923829 0.000009
 H14 3.793057 -0.303621 0.000005
 O15 0.131293 2.691433 -0.000004
 H16 -3.793757 -0.794611 -0.000008
 H17 0.889224 -2.343861 0.000006

Zero-point correction= 0.127827 (Hartree/Particle)
 Thermal correction to Energy= 0.136987
 Thermal correction to Enthalpy= 0.137931
 Thermal correction to Gibbs Free Energy= 0.093882
 Sum of electronic and zero-point Energies= -542.933691
 Sum of electronic and thermal Energies= -542.924531
 Sum of electronic and thermal Enthalpies= -542.923586
 Sum of electronic and thermal Free Energies= -542.967636

[G + H]⁺_11

C1 0.206066 1.328094 0.000014
 C2 -0.832507 0.434886 0.000019
 H3 2.232116 1.446015 -0.000544
 C4 1.696206 -0.581117 0.000044
 C5 -2.640924 -0.808462 0.000008
 N6 1.461261 0.785940 -0.000004
 N7 -2.217158 0.492237 0.000053
 N8 -1.670701 -1.692308 -0.000040
 N9 0.716104 -1.458743 0.000068
 C10 -0.521122 -0.964019 -0.000032

N11 2.972067 -0.995415 -0.000490
 H12 3.136392 -1.991559 0.000740
 H13 3.765978 -0.376180 0.002392
 O14 0.220439 2.655264 0.000010
 H15 -3.694494 -1.052129 0.000011
 H16 -2.821201 1.301244 0.000119
 H17 -0.659626 3.052222 -0.000229

Zero-point correction= 0.127606 (Hartree/Particle)
 Thermal correction to Energy= 0.136784
 Thermal correction to Enthalpy= 0.137728
 Thermal correction to Gibbs Free Energy= 0.093678
 Sum of electronic and zero-point Energies= -542.933550
 Sum of electronic and thermal Energies= -542.924371
 Sum of electronic and thermal Enthalpies= -542.923427
 Sum of electronic and thermal Free Energies= -542.967478

[G + H]⁺_12

C1 -0.195328 1.328505 -0.000418
 C2 0.826078 0.419481 0.000572
 H3 -2.253013 1.429226 -0.050732
 C4 -1.698805 -0.578553 0.002517
 C5 2.634606 -0.807677 0.000970
 N6 -1.460872 0.799354 -0.002299
 N7 2.204118 0.487068 0.004403
 N8 1.664672 -1.699465 -0.002251
 N9 -0.729036 -1.459458 0.003884
 C10 0.517147 -0.973868 -0.002765
 N11 -2.982295 -0.979322 -0.016310
 H12 -3.150907 -1.974512 0.016412
 H13 -3.767205 -0.361080 0.108256
 O14 0.013235 2.636480 -0.006217
 H15 3.688356 -1.049671 0.001013
 H16 2.781199 1.316712 0.004740
 H17 -0.782602 3.182904 0.052802

Zero-point correction= 0.127216 (Hartree/Particle)
 Thermal correction to Energy= 0.136582
 Thermal correction to Enthalpy= 0.137526
 Thermal correction to Gibbs Free Energy= 0.092964
 Sum of electronic and zero-point Energies= -542.931374
 Sum of electronic and thermal Energies= -542.922008
 Sum of electronic and thermal Enthalpies= -542.921063
 Sum of electronic and thermal Free Energies= -542.965625

[G + H]⁺_13

C1 -0.324016 1.495849 -0.000026
 C2 0.820646 0.544462 0.000025
 H3 -2.377458 1.378759 0.000008
 C4 -1.698695 -0.583447 0.000021
 H5 1.850308 -2.497602 0.000338
 C6 2.759701 -0.471303 0.000194
 N7 -1.555846 0.782061 0.000015
 N8 2.072304 0.797534 0.000046
 N9 1.704314 -1.495306 -0.000332
 N10 -0.674218 -1.450305 -0.000074
 C11 0.520180 -0.900893 -0.000140
 N12 -2.926212 -1.089071 0.000116
 H13 -3.024349 -2.095432 0.000091

H14 -3.761803 -0.523092 0.000193
 O15 -0.286063 2.688832 -0.000077
 H16 3.395729 -0.547982 0.889268
 H17 3.396784 -0.547711 -0.888118

Zero-point correction= 0.128249 (Hartree/Particle)
 Thermal correction to Energy= 0.136765
 Thermal correction to Enthalpy= 0.137709
 Thermal correction to Gibbs Free Energy= 0.094835
 Sum of electronic and zero-point Energies= -542.924227
 Sum of electronic and thermal Energies= -542.915711
 Sum of electronic and thermal Enthalpies= -542.914767
 Sum of electronic and thermal Free Energies= -542.957641

[G + H]⁺_14

C1 0.194206 1.354735 0.000000
 C2 -0.853752 0.420109 0.000002
 C3 1.606282 -0.404744 -0.000003
 C4 -2.682866 -0.647285 0.000001
 N5 1.456432 0.901115 -0.000002
 N6 -2.217884 0.575172 0.000003
 N7 -1.687841 -1.609129 -0.000001
 N8 0.761043 -1.406261 -0.000003
 C9 -0.499673 -0.938747 0.000000
 N10 3.044516 -0.829705 0.000003
 H11 3.095260 -1.853870 -0.000116
 H12 3.528534 -0.460966 -0.826225
 O13 0.028688 2.662442 -0.000001
 H14 -3.728468 -0.918375 0.000002
 H15 -0.916082 2.884250 0.000000
 H16 -1.816272 -2.612158 -0.000002
 H17 3.528475 -0.461171 0.826357

Zero-point correction= 0.130571 (Hartree/Particle)
 Thermal correction to Energy= 0.139063
 Thermal correction to Enthalpy= 0.140007
 Thermal correction to Gibbs Free Energy= 0.096742
 Sum of electronic and zero-point Energies= -542.923113
 Sum of electronic and thermal Energies= -542.914622
 Sum of electronic and thermal Enthalpies= -542.913678
 Sum of electronic and thermal Free Energies= -542.956943

[G + H]⁺_15

C1 0.196147 1.339366 -0.000002
 C2 -0.844582 0.409695 0.000004
 C3 1.597510 -0.427784 -0.000013
 C4 -2.644961 -0.840131 0.000004
 N5 1.455929 0.889470 -0.000011
 N6 -2.215449 0.461394 0.000009
 N7 -1.666780 -1.719531 -0.000004
 N8 0.747118 -1.409267 -0.000011
 C9 -0.533642 -0.969160 -0.000004
 N10 3.028638 -0.877224 0.000014
 H11 3.039173 -1.903658 -0.000348
 H12 3.525228 -0.530287 -0.827720
 O13 -0.055001 2.641525 0.000000
 H14 -3.696822 -1.087459 0.000007
 H15 -2.795247 1.289485 0.000016
 H16 0.773630 3.144816 -0.000003

H17 3.525016 -0.530908 0.828137

Zero-point correction= 0.130327 (Hartree/Particle)
 Thermal correction to Energy= 0.138834
 Thermal correction to Enthalpy= 0.139778
 Thermal correction to Gibbs Free Energy= 0.096689
 Sum of electronic and zero-point Energies= -542.922444
 Sum of electronic and thermal Energies= -542.913937
 Sum of electronic and thermal Enthalpies= -542.912993
 Sum of electronic and thermal Free Energies= -542.956082

[G + H]⁺_16

C1 0.218213 1.351398 -0.000007
 C2 -0.867087 0.457767 0.000027
 C3 1.583240 -0.456192 -0.000072
 C4 -2.715266 -0.577017 0.000031
 N5 1.469506 0.856680 -0.000055
 N6 -2.228182 0.634680 0.000055
 N7 -1.740410 -1.561211 -0.000019
 N8 0.703294 -1.421943 -0.000070
 C9 -0.542899 -0.913699 -0.000019
 N10 3.003509 -0.935036 0.000075
 H11 3.006617 -1.960799 -0.002168
 H12 3.505090 -0.590387 -0.825952
 O13 0.030428 2.653938 -0.000006
 H14 -3.766260 -0.826971 0.000050
 H15 0.882168 3.116855 -0.000022
 H16 -1.886002 -2.561722 -0.000043
 H17 3.503732 -0.594209 0.828516

Zero-point correction= 0.130364 (Hartree/Particle)
 Thermal correction to Energy= 0.138865
 Thermal correction to Enthalpy= 0.139809
 Thermal correction to Gibbs Free Energy= 0.096649
 Sum of electronic and zero-point Energies= -542.921343
 Sum of electronic and thermal Energies= -542.912842
 Sum of electronic and thermal Enthalpies= -542.911898
 Sum of electronic and thermal Free Energies= -542.955057

[G + H]⁺_17

C1 0.445295 1.339314 0.000000
 C2 -0.768951 0.516650 -0.000001
 C3 1.675713 -0.617269 0.000000
 C4 -2.746810 -0.414798 0.000002
 N5 1.606229 0.764991 0.000001
 N6 -2.009508 0.828327 -0.000006
 N7 -1.737644 -1.481965 0.000000
 N8 0.653568 -1.505294 0.000001
 C9 -0.525847 -0.936936 0.000000
 N10 2.902896 -1.107891 -0.000003
 H11 3.043452 -2.109069 0.000007
 H12 3.697337 -0.483603 0.000008
 O13 0.300788 2.638564 0.000000
 H14 -3.387464 -0.461494 0.888180
 H15 1.170821 3.074433 0.000000
 H16 -1.928152 -2.476214 -0.000012
 H17 -3.387493 -0.461509 -0.888152

Zero-point correction= 0.128661 (Hartree/Particle)

Thermal correction to Energy= 0.136955
 Thermal correction to Enthalpy= 0.137899
 Thermal correction to Gibbs Free Energy= 0.095492
 Sum of electronic and zero-point Energies= -542.917531
 Sum of electronic and thermal Energies= -542.909237
 Sum of electronic and thermal Enthalpies= -542.908293
 Sum of electronic and thermal Free Energies= -542.950700

[G + H]⁺_18

C1 0.418107 1.354034 0.000001
 C2 -0.759969 0.479160 -0.000079
 C3 1.706119 -0.556987 0.000031
 C4 -2.718568 -0.495949 0.000067
 N5 1.594424 0.820127 0.000093
 N6 -2.005477 0.765720 -0.000258
 N7 -1.681642 -1.536434 0.000018
 N8 0.716057 -1.489649 0.000143
 C9 -0.479537 -0.964452 0.000066
 N10 2.948281 -1.003566 -0.000249
 H11 3.127336 -1.998721 0.000229
 H12 3.716605 -0.346146 0.000242
 O13 0.295101 2.659698 0.000054
 H14 -3.357343 -0.558321 -0.888172
 H15 -0.637697 2.929675 -0.000036
 H16 -1.851694 -2.534453 -0.000491
 H17 -3.356428 -0.557831 0.889045

Zero-point correction= 0.128609 (Hartree/Particle)
 Thermal correction to Energy= 0.136949
 Thermal correction to Enthalpy= 0.137893
 Thermal correction to Gibbs Free Energy= 0.095411
 Sum of electronic and zero-point Energies= -542.913641
 Sum of electronic and thermal Energies= -542.905301
 Sum of electronic and thermal Enthalpies= -542.904357
 Sum of electronic and thermal Free Energies= -542.946839

[G + H]⁺_19

C1 0.063299 1.492746 0.000000
 C2 -0.887620 0.419504 0.000000
 H3 2.147533 1.612628 0.000003
 C4 1.622086 -0.416859 0.000000
 C5 -2.651135 -0.881149 0.000000
 N6 1.403955 0.922089 0.000002
 N7 -2.255181 0.427578 0.000000
 N8 -1.636948 -1.724346 0.000000
 N9 0.771591 -1.363152 -0.000001
 C10 -0.537826 -0.931530 0.000000
 N11 3.047660 -0.869931 -0.000001
 H12 3.003806 -1.898877 -0.000016
 H13 3.566017 -0.567030 -0.834430
 O14 -0.088777 2.686981 -0.000001
 H15 -3.693299 -1.163613 0.000001
 H16 -2.850204 1.246156 -0.000001
 H17 3.566008 -0.567055 0.834444

Zero-point correction= 0.129808 (Hartree/Particle)
 Thermal correction to Energy= 0.138369
 Thermal correction to Enthalpy= 0.139313
 Thermal correction to Gibbs Free Energy= 0.096267
 Sum of electronic and zero-point Energies= -542.903155

Sum of electronic and thermal Energies= -542.894594
 Sum of electronic and thermal Enthalpies= -542.893649
 Sum of electronic and thermal Free Energies= -542.936696

[G + H]⁺_20

C1 -0.292891 1.470867 -0.000003
 C2 0.796389 0.456721 -0.000005
 H3 -2.324593 1.454852 0.000035
 C4 -1.716562 -0.563803 -0.000003
 C5 2.699445 -0.726120 0.000003
 N6 -1.521981 0.833047 -0.000003
 N7 2.073349 0.628624 -0.000002
 N8 1.627065 -1.653532 0.000003
 N9 -0.755471 -1.449591 -0.000008
 C10 0.508226 -0.981166 -0.000001
 N11 -2.991603 -0.967129 0.000032
 H12 -3.166892 -1.962299 -0.000037
 H13 -3.779835 -0.339504 -0.000128
 O14 -0.116749 2.661464 0.000003
 H15 3.334868 -0.826947 -0.889571
 H16 2.548432 1.530201 -0.000003
 H17 3.334863 -0.826941 0.889581

Zero-point correction= 0.127110 (Hartree/Particle)
 Thermal correction to Energy= 0.135806
 Thermal correction to Enthalpy= 0.136750
 Thermal correction to Gibbs Free Energy= 0.093538
 Sum of electronic and zero-point Energies= -542.899465
 Sum of electronic and thermal Energies= -542.890769
 Sum of electronic and thermal Enthalpies= -542.889825
 Sum of electronic and thermal Free Energies= -542.933037

[G + H]⁺_21

C1 0.079952 1.519438 0.000000
 C2 -0.922494 0.475710 0.000000
 H3 2.181271 1.562742 0.000003
 C4 1.612691 -0.444121 0.000000
 H5 -1.806441 -2.579397 0.000000
 C6 -2.726048 -0.642224 0.000001
 N7 1.421350 0.889888 0.000002
 N8 -2.282406 0.591495 0.000001
 N9 -1.710339 -1.572822 0.000000
 N10 0.728199 -1.369428 -0.000002
 C11 -0.543538 -0.866014 -0.000001
 N12 3.023926 -0.934234 0.000000
 H13 2.967683 -1.961635 -0.000027
 H14 3.548031 -0.638238 -0.833738
 O15 0.007315 2.712265 -0.000002
 H16 -3.765558 -0.934338 0.000002
 H17 3.548011 -0.638282 0.833767

Zero-point correction= 0.129464 (Hartree/Particle)
 Thermal correction to Energy= 0.138088
 Thermal correction to Enthalpy= 0.139032
 Thermal correction to Gibbs Free Energy= 0.095856
 Sum of electronic and zero-point Energies= -542.896953
 Sum of electronic and thermal Energies= -542.888329
 Sum of electronic and thermal Enthalpies= -542.887384
 Sum of electronic and thermal Free Energies= -542.930561

[G + H]⁺_22

C1 0.227539 1.456886 -0.000005
 C2 -0.763398 0.432357 -0.000014
 H3 2.289903 1.491906 0.000021
 C4 1.747974 -0.515441 -0.000003
 C5 -2.625523 -0.918750 0.000007
 N6 1.515699 0.835360 -0.000008
 N7 -2.211463 0.564641 0.000002
 N8 -1.642484 -1.697142 0.000000
 N9 0.764380 -1.422946 -0.000006
 C10 -0.449023 -0.905172 -0.000009
 N11 3.009035 -0.955546 0.000054
 H12 3.158940 -1.954213 -0.000108
 H13 3.810895 -0.345332 -0.000142
 O14 0.089280 2.658753 0.000006
 H15 -3.684220 -1.143959 0.000019
 H16 -2.580678 1.055865 -0.826934
 H17 -2.580660 1.055861 0.826949

Zero-point correction= 0.128263 (Hartree/Particle)
 Thermal correction to Energy= 0.136946
 Thermal correction to Enthalpy= 0.137890
 Thermal correction to Gibbs Free Energy= 0.094651
 Sum of electronic and zero-point Energies= -542.889391
 Sum of electronic and thermal Energies= -542.880708
 Sum of electronic and thermal Enthalpies= -542.879764
 Sum of electronic and thermal Free Energies= -542.923003

[G + H]⁺_23

C1 0.392755 1.329706 0.000007
 C2 -0.761011 0.441000 -0.000061
 C3 1.706441 -0.592576 0.000025
 C4 -2.689885 -0.702546 -0.000002
 N5 1.565398 0.815128 0.000100
 N6 -2.040445 0.639691 -0.000091
 N7 -1.641295 -1.652983 0.000032
 N8 0.746076 -1.493345 0.000147
 C9 -0.503367 -1.005796 0.000050
 N10 2.982080 -0.978352 -0.000246
 H11 3.201425 -1.964311 -0.000183
 H12 3.722775 -0.294269 0.000390
 O13 0.140159 2.629026 0.000042
 H14 -3.328265 -0.792037 0.889188
 H15 -2.509531 1.542153 -0.000515
 H16 0.968517 3.138676 0.000087
 H17 -3.328483 -0.792128 -0.889013

Zero-point correction= 0.127209 (Hartree/Particle)
 Thermal correction to Energy= 0.135637
 Thermal correction to Enthalpy= 0.136581
 Thermal correction to Gibbs Free Energy= 0.093974
 Sum of electronic and zero-point Energies= -542.887989
 Sum of electronic and thermal Energies= -542.879561
 Sum of electronic and thermal Enthalpies= -542.878617
 Sum of electronic and thermal Free Energies= -542.921224

[G + H]⁺_24

C1 0.405418 1.331510 0.000002
 C2 -0.752501 0.519801 0.000002

C3 1.705025 -0.583455 -0.000001
 C4 -2.761581 -0.293437 -0.000010
 N5 1.599110 0.761050 -0.000001
 N6 -2.123160 0.793977 -0.000005
 N7 -1.812988 -1.509832 0.000005
 N8 0.650470 -1.462284 0.000001
 C9 -0.482376 -0.835148 0.000003
 N10 2.930847 -1.113710 0.000019
 H11 3.050897 -2.114320 -0.000079
 H12 3.737994 -0.509625 -0.000078
 O13 0.292989 2.643636 0.000002
 H14 -3.825576 -0.479849 -0.000018
 H15 1.177738 3.043779 0.000002
 H16 -1.939416 -2.104536 0.828286
 H17 -1.939410 -2.104580 -0.828246

Zero-point correction= 0.128234 (Hartree/Particle)
 Thermal correction to Energy= 0.136706
 Thermal correction to Enthalpy= 0.137650
 Thermal correction to Gibbs Free Energy= 0.095048
 Sum of electronic and zero-point Energies= -542.887704
 Sum of electronic and thermal Energies= -542.879233
 Sum of electronic and thermal Enthalpies= -542.878289
 Sum of electronic and thermal Free Energies= -542.920891

[G + H]⁺_25

C1 -0.286049 1.496249 0.000097
 C2 0.800429 0.536033 0.000168
 H3 -2.352382 1.397862 0.000002
 C4 -1.719888 -0.569393 -0.000030
 H5 1.874661 -2.123943 0.829308
 C6 2.776894 -0.355040 -0.000453
 N7 -1.546260 0.780761 0.000056
 N8 2.181611 0.755566 -0.000189
 N9 1.775688 -1.524631 0.000293
 N10 -0.678270 -1.418704 0.000043
 C11 0.477594 -0.792526 0.000107
 N12 -2.954418 -1.080896 -0.000196
 H13 -3.058261 -2.084711 -0.000288
 H14 -3.785606 -0.510825 -0.000303
 O15 -0.265871 2.694566 0.000070
 H16 3.832057 -0.586573 -0.000609
 H17 1.874164 -2.124955 -0.828053

Zero-point correction= 0.127853 (Hartree/Particle)
 Thermal correction to Energy= 0.136546
 Thermal correction to Enthalpy= 0.137490
 Thermal correction to Gibbs Free Energy= 0.094376
 Sum of electronic and zero-point Energies= -542.886735
 Sum of electronic and thermal Energies= -542.878042
 Sum of electronic and thermal Enthalpies= -542.877098
 Sum of electronic and thermal Free Energies= -542.920212

[G + H]⁺_26

C1 -0.348324 1.307104 0.000001
 C2 0.731120 0.425193 0.000005
 C3 -1.738445 -0.527700 0.000000
 C4 2.630769 -0.888073 -0.000002
 N5 -1.571442 0.818414 0.000000

N6 2.177862 0.597199 0.000002
 N7 1.670779 -1.690710 -0.000002
 N8 -0.739968 -1.458904 0.000000
 C9 0.452836 -0.937797 0.000001
 N10 -2.990145 -0.991349 0.000001
 H11 -3.152718 -1.986455 -0.000003
 H12 -3.768702 -0.351488 -0.000003
 O13 -0.133560 2.619826 -0.000002
 H14 3.696239 -1.078466 -0.000003
 H15 2.541049 1.088730 -0.828100
 H16 -0.985771 3.085432 -0.000004
 H17 2.541053 1.088728 0.828102

Zero-point correction= 0.128429 (Hartree/Particle)
 Thermal correction to Energy= 0.136924
 Thermal correction to Enthalpy= 0.137868
 Thermal correction to Gibbs Free Energy= 0.095120
 Sum of electronic and zero-point Energies= -542.884751
 Sum of electronic and thermal Energies= -542.876257
 Sum of electronic and thermal Enthalpies= -542.875313
 Sum of electronic and thermal Free Energies= -542.918060

[G + H]⁺_27

C1 0.383936 1.344028 0.000000
 C2 -0.745906 0.490236 0.000000
 C3 1.731439 -0.530137 0.000000
 C4 -2.737580 -0.369299 0.000000
 N5 1.588760 0.807524 -0.000001
 N6 -2.119818 0.733419 0.000000
 N7 -1.763911 -1.559732 0.000000
 N8 0.703842 -1.450345 0.000000
 C9 -0.443247 -0.857923 0.000000
 N10 2.971755 -1.022921 -0.000001
 H11 3.125579 -2.018894 0.000004
 H12 3.756830 -0.389466 0.000004
 O13 0.310461 2.664008 0.000000
 H14 -3.797740 -0.575468 0.000000
 H15 -0.608330 2.969653 0.000003
 H16 -1.878138 -2.157469 0.828165
 H17 -1.878137 -2.157470 -0.828164

Zero-point correction= 0.128120 (Hartree/Particle)
 Thermal correction to Energy= 0.136626
 Thermal correction to Enthalpy= 0.137570
 Thermal correction to Gibbs Free Energy= 0.094909
 Sum of electronic and zero-point Energies= -542.882044
 Sum of electronic and thermal Energies= -542.873538
 Sum of electronic and thermal Enthalpies= -542.872593
 Sum of electronic and thermal Free Energies= -542.915254

[G + H]⁺_28

C1 -0.304887 1.182079 -0.017928
 C2 0.827941 0.420286 -0.014499
 C3 -1.710599 -0.578208 0.001033
 C4 2.684258 -0.580694 0.007863
 N5 -1.524270 0.783567 -0.003458
 N6 2.188032 0.628346 -0.003358
 N7 1.721103 -1.577587 0.005988
 N8 -0.714559 -1.481927 0.000040

C9 0.497677 -0.963748 -0.003746
 N10 -2.978191 -1.016282 0.011398
 H11 -3.158859 -2.007428 0.005087
 H12 -3.746255 -0.366245 -0.011003
 O13 -0.159607 2.673965 -0.064330
 H14 3.738247 -0.816851 0.018522
 H15 -0.944617 3.134699 0.296492
 H16 1.884580 -2.575708 0.011632
 H17 0.692615 3.008708 0.283306

Zero-point correction= 0.127062 (Hartree/Particle)
 Thermal correction to Energy= 0.136044
 Thermal correction to Enthalpy= 0.136988
 Thermal correction to Gibbs Free Energy= 0.093482
 Sum of electronic and zero-point Energies= -542.880709
 Sum of electronic and thermal Energies= -542.871726
 Sum of electronic and thermal Enthalpies= -542.870782
 Sum of electronic and thermal Free Energies= -542.914289

[G + H]⁺_29

C1 0.321395 1.165573 -0.000968
 C2 -0.824235 0.435847 -0.004633
 C3 1.687728 -0.630775 0.001159
 C4 -2.667583 -0.754112 -0.014844
 N5 1.532315 0.732809 -0.004536
 N6 -2.197288 0.541108 -0.023190
 N7 -1.735534 -1.667656 0.018004
 N8 0.668388 -1.498173 0.025507
 C9 -0.547151 -0.984269 0.020809
 N10 2.943000 -1.106331 -0.014538
 H11 3.087239 -2.103787 -0.008590
 H12 3.733851 -0.484470 -0.027493
 O13 0.263229 2.706293 -0.035863
 H14 -3.729616 -0.956184 -0.032891
 H15 -2.760643 1.374213 -0.108534
 H16 1.119270 3.014977 -0.405684
 H17 0.146978 3.099015 0.852232

Zero-point correction= 0.125951 (Hartree/Particle)
 Thermal correction to Energy= 0.135360
 Thermal correction to Enthalpy= 0.136304
 Thermal correction to Gibbs Free Energy= 0.091695
 Sum of electronic and zero-point Energies= -542.860689
 Sum of electronic and thermal Energies= -542.851281
 Sum of electronic and thermal Enthalpies= -542.850336
 Sum of electronic and thermal Free Energies= -542.894945

Cartesian coordinates for the structures of deprotonated guanine tautomers in Fig. S2, optimized at B3LYP/6-311++G**

[G – H]⁻_1

C1 -0.261745 1.428800 -0.003263
 C2 0.765510 0.419349 -0.012580
 C3 -1.691904 -0.435350 -0.016907
 C4 2.615347 -0.772707 0.010356
 N5 -1.529603 0.896650 -0.006352
 N6 2.145362 0.509748 -0.000700
 N7 1.656002 -1.677019 0.007815
 N8 -0.788039 -1.421224 -0.007000
 C9 0.477926 -0.939952 -0.006224
 N10 -3.034318 -0.859181 -0.073907
 H11 -3.161090 -1.784758 0.310988
 H12 -3.665539 -0.165557 0.301187
 O13 -0.011434 2.653556 0.012729
 H14 3.674006 -0.992731 0.018040
 H15 2.667459 1.370943 0.000678

Zero-point correction= 0.102986 (Hartree/Particle)
 Thermal correction to Energy= 0.110993
 Thermal correction to Enthalpy= 0.111938
 Thermal correction to Gibbs Free Energy= 0.070107
 Sum of electronic and zero-point Energies= -542.062770
 Sum of electronic and thermal Energies= -542.054763
 Sum of electronic and thermal Enthalpies= -542.053819
 Sum of electronic and thermal Free Energies= -542.095650

[G – H]⁻_2

C1 -0.136183 1.449359 0.003059
 C2 0.893875 0.465458 0.015337
 H3 -2.198608 1.443610 -0.134905
 C4 -1.642655 -0.546174 -0.010970
 C5 2.666757 -0.671313 0.004152
 N6 -1.422639 0.810027 -0.003705
 N7 2.260333 0.601259 0.019901
 N8 1.710326 -1.641755 -0.010623
 N9 -0.710083 -1.438173 0.001283
 C10 0.573258 -0.920038 -0.005602
 N11 -3.002840 -0.930882 -0.074502
 H12 -3.053462 -1.939212 0.010961
 H13 -3.568343 -0.494541 0.646387
 O14 -0.109534 2.681566 -0.011080
 H15 3.720698 -0.929466 0.003874

Zero-point correction= 0.103109 (Hartree/Particle)
 Thermal correction to Energy= 0.111113
 Thermal correction to Enthalpy= 0.112058
 Thermal correction to Gibbs Free Energy= 0.070171
 Sum of electronic and zero-point Energies= -542.062095
 Sum of electronic and thermal Energies= -542.054091
 Sum of electronic and thermal Enthalpies= -542.053147
 Sum of electronic and thermal Free Energies= -542.095034

[G – H]⁻_3

C1 -0.208920 1.293362 -0.005712
 C2 0.836608 0.380929 -0.012015

C3 -1.683837 -0.443153 -0.015907
 C4 2.597156 -0.758598 0.010025
 N5 -1.473133 0.896948 -0.008769
 N6 2.205505 0.525632 -0.000369
 N7 1.639938 -1.723783 0.008266
 N8 -0.794472 -1.424685 -0.005082
 C9 0.494264 -0.996279 -0.006333
 N10 -3.040109 -0.818431 -0.074654
 H11 -3.189638 -1.749809 0.287476
 H12 -3.649958 -0.123280 0.332178
 O13 0.027785 2.640106 0.011216
 H14 3.649755 -1.022905 0.019207
 H15 0.991841 2.727816 0.015317

Zero-point correction= 0.103532 (Hartree/Particle)
 Thermal correction to Energy= 0.111383
 Thermal correction to Enthalpy= 0.112327
 Thermal correction to Gibbs Free Energy= 0.070853
 Sum of electronic and zero-point Energies= -542.060790
 Sum of electronic and thermal Energies= -542.052939
 Sum of electronic and thermal Enthalpies= -542.051995
 Sum of electronic and thermal Free Energies= -542.093469

[G – H]⁻_4

C1 -0.310330 1.440830 -0.000033
 C2 0.791396 0.517963 -0.000027
 H3 -2.360139 1.315978 0.000150
 C4 -1.762014 -0.651156 0.000000
 H5 1.878931 -2.463553 0.000043
 C6 2.691992 -0.460442 0.000057
 N7 -1.527740 0.743846 -0.000227
 N8 2.162495 0.730938 0.000053
 N9 1.732534 -1.467531 -0.000021
 N10 -0.678469 -1.489169 -0.000060
 C11 0.491412 -0.855702 -0.000058
 N12 -3.013151 -1.015163 0.000192
 H13 -3.032147 -2.033030 -0.000051
 O14 -0.297580 2.674251 0.000072
 H15 3.749568 -0.682806 0.000102

Zero-point correction= 0.102612 (Hartree/Particle)
 Thermal correction to Energy= 0.110635
 Thermal correction to Enthalpy= 0.111579
 Thermal correction to Gibbs Free Energy= 0.069553
 Sum of electronic and zero-point Energies= -542.060007
 Sum of electronic and thermal Energies= -542.051984
 Sum of electronic and thermal Enthalpies= -542.051040
 Sum of electronic and thermal Free Energies= -542.093066

[G – H]⁻_5

C1 -0.300398 1.453696 -0.002495
 C2 0.805283 0.502149 -0.005665
 C3 -1.673616 -0.476007 -0.017314
 H4 1.842917 -2.505125 -0.002611
 C5 2.690376 -0.520092 0.006928
 N6 -1.555969 0.844303 -0.006930
 N7 2.183859 0.683800 0.002188
 N8 1.714645 -1.506625 0.005506
 N9 -0.718215 -1.429144 -0.007641

C10 0.496071 -0.856066 -0.004003
 N11 -2.991074 -0.969699 -0.074137
 H12 -3.080977 -1.888388 0.336792
 H13 -3.657286 -0.295257 0.274696
 O14 -0.173386 2.684124 0.010198
 H15 3.743418 -0.764740 0.011929

Zero-point correction= 0.102655 (Hartree/Particle)
 Thermal correction to Energy= 0.110735
 Thermal correction to Enthalpy= 0.111679
 Thermal correction to Gibbs Free Energy= 0.069690
 Sum of electronic and zero-point Energies= -542.058703
 Sum of electronic and thermal Energies= -542.050623
 Sum of electronic and thermal Enthalpies= -542.049679
 Sum of electronic and thermal Free Energies= -542.091668

[G - H]_6

C1 -0.249306 1.285681 -0.003756
 C2 0.858541 0.451072 -0.007597
 C3 -1.632167 -0.547745 -0.016468
 C4 2.662567 -0.623142 0.009478
 N5 -1.492257 0.798300 -0.009404
 N6 2.223245 0.639461 0.002690
 N7 1.746992 -1.631354 0.005993
 N8 -0.681792 -1.464095 -0.005991
 C9 0.577312 -0.954249 -0.005741
 N10 -2.964590 -1.005320 -0.075852
 H11 -3.046394 -1.950012 0.274270
 H12 -3.612945 -0.363339 0.358503
 O13 -0.141585 2.646168 0.009315
 H14 3.725502 -0.844580 0.017149
 H15 -1.056349 2.959941 -0.001988

Zero-point correction= 0.103232 (Hartree/Particle)
 Thermal correction to Energy= 0.111128
 Thermal correction to Enthalpy= 0.112072
 Thermal correction to Gibbs Free Energy= 0.070523
 Sum of electronic and zero-point Energies= -542.058127
 Sum of electronic and thermal Energies= -542.050231
 Sum of electronic and thermal Enthalpies= -542.049287
 Sum of electronic and thermal Free Energies= -542.090837

[G - H]_7

C1 -0.271114 1.418413 -0.000075
 C2 0.754253 0.438205 -0.000218
 H3 -2.324507 1.391218 0.000424
 C4 -1.787477 -0.605081 -0.000024
 C5 2.620039 -0.719260 0.000149
 N6 -1.510363 0.793390 -0.000363
 N7 2.138323 0.555063 0.000034
 N8 1.681395 -1.640911 0.000052
 N9 -0.746020 -1.486212 -0.000116
 C10 0.472776 -0.937175 -0.000131
 N11 -3.057548 -0.905303 0.000299
 H12 -3.124898 -1.920937 0.000158
 O13 -0.145264 2.656340 0.000193
 H14 3.682869 -0.921014 0.000281
 H15 2.657282 1.417223 0.000052

Zero-point correction= 0.102374 (Hartree/Particle)
 Thermal correction to Energy= 0.110558
 Thermal correction to Enthalpy= 0.111502
 Thermal correction to Gibbs Free Energy= 0.069050
 Sum of electronic and zero-point Energies= -542.054890
 Sum of electronic and thermal Energies= -542.046706
 Sum of electronic and thermal Enthalpies= -542.045762
 Sum of electronic and thermal Free Energies= -542.088214

[G - H]_8

C1 -0.325702 1.426675 -0.000008
 C2 0.789492 0.529305 -0.000037
 H3 -2.353635 1.288925 0.000168
 C4 -1.748019 -0.713224 -0.000004
 H5 1.923166 -2.434772 0.000073
 C6 2.704287 -0.418747 0.000001
 N7 -1.533554 0.699137 -0.000019
 N8 2.157783 0.764736 -0.000036
 N9 1.762370 -1.440895 0.000025
 N10 -0.640560 -1.511129 0.000013
 C11 0.509307 -0.851083 0.000007
 N12 -2.953860 -1.211350 -0.000011
 H13 -3.639650 -0.456750 -0.000080
 O14 -0.352099 2.660674 0.000034
 H15 3.765459 -0.623845 0.000004

Zero-point correction= 0.102056 (Hartree/Particle)
 Thermal correction to Energy= 0.110162
 Thermal correction to Enthalpy= 0.111106
 Thermal correction to Gibbs Free Energy= 0.068928
 Sum of electronic and zero-point Energies= -542.051739
 Sum of electronic and thermal Energies= -542.043633
 Sum of electronic and thermal Enthalpies= -542.042689
 Sum of electronic and thermal Free Energies= -542.084867

[G - H]_9

C1 -0.288779 1.404223 -0.000021
 C2 0.753125 0.450146 -0.000227
 H3 -2.319612 1.363467 0.000465
 C4 -1.775889 -0.671056 -0.000002
 C5 2.637934 -0.675638 0.000058
 N6 -1.519404 0.747124 0.000030
 N7 2.135995 0.591561 -0.000137
 N8 1.717704 -1.613192 0.000135
 N9 -0.706296 -1.510995 0.000065
 C10 0.493200 -0.932234 -0.000008
 N11 -3.006736 -1.109918 -0.000086
 H12 -3.656152 -0.323505 -0.000205
 O13 -0.204586 2.646580 0.000124
 H14 3.704351 -0.858672 0.000109
 H15 2.641719 1.461364 -0.000210

Zero-point correction= 0.101577 (Hartree/Particle)
 Thermal correction to Energy= 0.109916
 Thermal correction to Enthalpy= 0.110861
 Thermal correction to Gibbs Free Energy= 0.068087
 Sum of electronic and zero-point Energies= -542.044681
 Sum of electronic and thermal Energies= -542.036342
 Sum of electronic and thermal Enthalpies= -542.035397
 Sum of electronic and thermal Free Energies= -542.078171

[G - H]_10

C1 0.409120 1.280180 -0.000004
 C2 -0.764684 0.501164 0.000157
 C3 1.770782 -0.647886 -0.000025
 C4 -2.690358 -0.419901 0.000087
 N5 1.598144 0.751032 -0.000139
 N6 -2.129881 0.758918 0.000244
 N7 -1.763475 -1.459212 -0.000187
 N8 0.660148 -1.503925 -0.000225
 C9 -0.498638 -0.885028 -0.000082
 N10 2.994128 -1.100660 0.000306
 H11 2.926006 -2.118643 0.000193
 O12 0.330632 2.645120 -0.000113
 H13 -3.754309 -0.609516 0.000128
 H14 1.259465 2.921619 -0.000167
 H15 -1.946999 -2.448676 -0.000050

Zero-point correction= 0.101952 (Hartree/Particle)
 Thermal correction to Energy= 0.110081
 Thermal correction to Enthalpy= 0.111025
 Thermal correction to Gibbs Free Energy= 0.068765
 Sum of electronic and zero-point Energies= -542.027066
 Sum of electronic and thermal Energies= -542.018937
 Sum of electronic and thermal Enthalpies= -542.017993
 Sum of electronic and thermal Free Energies= -542.060253

[G - H]_11

C1 -0.439107 1.255616 -0.000004
 C2 0.754339 0.513400 -0.000180
 C3 -1.736939 -0.732943 0.000003
 C4 2.705556 -0.350314 -0.000037
 N5 -1.611119 0.682279 0.000106
 N6 2.111740 0.812047 -0.000184
 N7 1.811589 -1.416631 0.000143
 N8 -0.603657 -1.542779 0.000197
 C9 0.528275 -0.882392 0.000025
 N10 -2.919480 -1.283925 -0.000234
 H11 -3.599180 -0.524378 -0.000029
 O12 -0.406585 2.622927 0.000103
 H13 3.774877 -0.507549 -0.000023
 H14 -1.342598 2.871911 0.000173
 H15 2.023324 -2.400541 0.000022

Zero-point correction= 0.101936 (Hartree/Particle)
 Thermal correction to Energy= 0.110066
 Thermal correction to Enthalpy= 0.111010
 Thermal correction to Gibbs Free Energy= 0.068763
 Sum of electronic and zero-point Energies= -542.026497
 Sum of electronic and thermal Energies= -542.018368
 Sum of electronic and thermal Enthalpies= -542.017424
 Sum of electronic and thermal Free Energies= -542.059671

[G - H]_12

C1 -0.400921 1.275536 -0.000016
 C2 0.741774 0.450301 -0.000206
 C3 -1.798056 -0.626259 0.000003
 C4 2.656094 -0.490345 0.000012
 N5 -1.599076 0.785442 0.000106
 N6 2.106294 0.698047 -0.000133

N7 1.714359 -1.514850 0.000100
 N8 -0.717963 -1.513980 0.000121
 C9 0.451724 -0.925707 -0.000023
 N10 -3.010170 -1.104824 -0.000130
 H11 -3.640616 -0.304105 -0.000098
 O12 -0.252733 2.643027 0.000101
 H13 3.717256 -0.692262 0.000054
 H14 0.699225 2.808475 0.000055
 H15 1.888206 -2.506325 0.000113

Zero-point correction= 0.101836 (Hartree/Particle)
 Thermal correction to Energy= 0.110066
 Thermal correction to Enthalpy= 0.111010
 Thermal correction to Gibbs Free Energy= 0.068516
 Sum of electronic and zero-point Energies= -542.023788
 Sum of electronic and thermal Energies= -542.015558
 Sum of electronic and thermal Enthalpies= -542.014614
 Sum of electronic and thermal Free Energies= -542.057107

[G - H]_13

C1 0.362871 1.301938 0.000004
 C2 -0.752789 0.434906 0.000272
 C3 1.830675 -0.527231 -0.000033
 C4 -2.633862 -0.572557 0.000068
 N5 1.577980 0.864023 -0.000191
 N6 -2.124768 0.633856 0.000302
 N7 -1.655038 -1.563214 -0.000209
 N8 0.780789 -1.465923 -0.000273
 C9 -0.416129 -0.927989 -0.000057
 N10 3.078380 -0.903563 0.000339
 H11 3.072305 -1.924026 0.000297
 O12 0.157934 2.662165 -0.000170
 H13 -3.687012 -0.812338 0.000071
 H14 -0.799922 2.788354 -0.000112
 H15 -1.794838 -2.559965 -0.000198

Zero-point correction= 0.101762 (Hartree/Particle)
 Thermal correction to Energy= 0.110008
 Thermal correction to Enthalpy= 0.110952
 Thermal correction to Gibbs Free Energy= 0.068414
 Sum of electronic and zero-point Energies= -542.023130
 Sum of electronic and thermal Energies= -542.014884
 Sum of electronic and thermal Enthalpies= -542.013939
 Sum of electronic and thermal Free Energies= -542.056478

[G - H]_14

C1 0.377023 1.268466 0.000842
 C2 -0.739404 0.435533 0.014969
 C3 1.798917 -0.604146 -0.000404
 C4 -2.627239 -0.694504 -0.002523
 N5 1.584924 0.796525 -0.004490
 N6 -2.126690 0.578605 0.001871
 N7 -1.712234 -1.633472 -0.006941
 N8 0.721666 -1.494395 -0.007138
 C9 -0.481321 -0.952737 0.001386
 N10 3.041005 -1.007899 0.007361
 H11 3.010268 -2.027498 0.008566
 O12 0.210534 2.637169 -0.006224
 H13 -3.694660 -0.873283 -0.003127

H14 -2.647471 1.437726 0.038991
 H15 1.119059 2.974476 -0.014909

Zero-point correction= 0.101148 (Hartree/Particle)
 Thermal correction to Energy= 0.109759
 Thermal correction to Enthalpy= 0.110703
 Thermal correction to Gibbs Free Energy= 0.066588
 Sum of electronic and zero-point Energies= -542.016721
 Sum of electronic and thermal Energies= -542.008109
 Sum of electronic and thermal Enthalpies= -542.007165
 Sum of electronic and thermal Free Energies= -542.051280

[G - H]_15

C1 0.408065 1.244006 0.001454
 C2 -0.730027 0.447602 0.033777
 C3 1.767953 -0.692047 -0.000971
 C4 -2.651157 -0.624145 -0.004836
 N5 1.601119 0.726477 -0.011508
 N6 -2.112790 0.634606 0.004824
 N7 -1.768113 -1.590686 -0.016045
 N8 0.664656 -1.536494 -0.016903
 C9 -0.513243 -0.950553 0.002684
 N10 2.972627 -1.197403 0.018286
 H11 3.623606 -0.412980 0.023167
 O12 0.288696 2.618132 -0.014679
 H13 -3.723878 -0.769214 -0.005687
 H14 -2.607762 1.505273 0.092749
 H15 1.206425 2.927182 -0.036032

Zero-point correction= 0.101104 (Hartree/Particle)
 Thermal correction to Energy= 0.109642
 Thermal correction to Enthalpy= 0.110586
 Thermal correction to Gibbs Free Energy= 0.067082
 Sum of electronic and zero-point Energies= -542.014282
 Sum of electronic and thermal Energies= -542.005743
 Sum of electronic and thermal Enthalpies= -542.004799
 Sum of electronic and thermal Free Energies= -542.048304

Cartesian coordinates for the structures of monohydrated protonated guanine tautomers in Fig. S3, optimized at B3LYP/6-311++G**

[G + H]⁺_1^{••}W67

C1 0.098254 -1.214955 -0.000014
 C2 0.476107 0.169422 -0.000010
 H3 -1.658902 -2.268938 -0.000009
 C4 -2.203327 -0.258881 0.000005
 H5 -0.213982 3.277855 0.000010
 C6 1.531476 2.094252 -0.000009
 N7 -1.314447 -1.314887 -0.000008
 N8 1.713577 0.784997 -0.000018
 N9 0.205286 2.356192 0.000002
 N10 -1.817462 1.007832 0.000010
 C11 -0.492196 1.157823 0.000001
 N12 -3.514712 -0.543301 0.000010
 H13 -4.166581 0.226330 0.000024
 H14 -3.877151 -1.482493 0.000019
 O15 0.807243 -2.203154 -0.000022
 H16 2.310372 2.839053 -0.000010
 H17 2.609109 0.244173 -0.000021
 O18 3.488719 -1.184534 0.000060
 H19 2.872127 -1.934834 0.000019
 H20 4.389743 -1.521436 -0.000141

Zero-point correction= 0.153660 (Hartree/Particle)
 Thermal correction to Energy= 0.165330
 Thermal correction to Enthalpy= 0.166274
 Thermal correction to Gibbs Free Energy= 0.116289
 Sum of electronic and zero-point Energies= -619.423038
 Sum of electronic and thermal Energies= -619.411367
 Sum of electronic and thermal Enthalpies= -619.410423
 Sum of electronic and thermal Free Energies= -619.460409

[G + H]⁺_1^{••}W9

C1 1.758691 -1.007360 -0.000004
 C2 0.322070 -1.046985 0.000009
 H3 3.186451 0.468427 -0.000008
 C4 1.354532 1.456568 -0.000008
 H5 -2.585803 0.343383 0.000005
 C6 -1.808138 -1.615966 0.000009
 N7 2.179030 0.351689 -0.000011
 N8 -0.569134 -2.104134 0.000009
 N9 -1.753175 -0.276245 0.000006
 N10 0.033303 1.374590 -0.000003
 C11 -0.422906 0.118267 0.000004
 N12 1.933158 2.669185 -0.000006
 H13 1.334001 3.479965 -0.000016
 H14 2.930442 2.805031 -0.000035
 O15 2.541529 -1.928295 -0.000008
 H16 -2.712812 -2.201496 0.000011
 H17 -0.317913 -3.085725 0.000011
 O18 -4.131392 1.128810 0.000007
 H19 -4.551612 1.526789 -0.771199
 H20 -4.551621 1.526772 0.771217

Zero-point correction= 0.153131 (Hartree/Particle)

Thermal correction to Energy= 0.165439
 Thermal correction to Enthalpy= 0.166383
 Thermal correction to Gibbs Free Energy= 0.114183
 Sum of electronic and zero-point Energies= -619.419466
 Sum of electronic and thermal Energies= -619.407157
 Sum of electronic and thermal Enthalpies= -619.406213
 Sum of electronic and thermal Free Energies= -619.458413

[G + H]⁺_1^{••}W12

C1 0.085947 1.284230 -0.000056
 C2 -1.170423 0.578412 -0.000008
 H3 2.088576 0.730651 -0.000121
 C4 1.005993 -1.027987 -0.000056
 H5 -2.913347 -2.091467 0.000078
 C6 -3.296427 -0.024474 0.000064
 N7 1.141674 0.343407 -0.000076
 N8 -2.479360 1.023533 0.000026
 N9 -2.551108 -1.145538 0.000056
 N10 -0.172919 -1.646701 -0.000013
 C11 -1.201955 -0.804359 0.000010
 N12 2.131354 -1.751356 -0.000075
 H13 2.052977 -2.756148 -0.000092
 H14 3.040896 -1.305707 -0.000137
 O15 0.268018 2.480862 -0.000078
 H16 -4.373187 0.013924 0.000096
 H17 -2.767454 1.995595 0.000021
 O18 4.069487 0.517246 0.000124
 H19 4.572370 0.814866 0.768427
 H20 4.572828 0.815079 -0.767796

Zero-point correction= 0.154643 (Hartree/Particle)
 Thermal correction to Energy= 0.166214
 Thermal correction to Enthalpy= 0.167158
 Thermal correction to Gibbs Free Energy= 0.117155
 Sum of electronic and zero-point Energies= -619.418265
 Sum of electronic and thermal Energies= -619.406695
 Sum of electronic and thermal Enthalpies= -619.405751
 Sum of electronic and thermal Free Energies= -619.455753

[G + H]⁺_1^{••}W16

C1 0.458725 -1.006176 0.000026
 C2 -0.934160 -0.647789 -0.000010
 H3 2.259532 -0.023677 0.000045
 C4 0.767192 1.451774 -0.000009
 H5 -3.294388 1.497047 -0.000096
 C6 -3.143240 -0.599438 -0.000057
 N7 1.244930 0.165276 0.000022
 N8 -2.089097 -1.408540 -0.000021
 N9 -2.705076 0.673028 -0.000070
 N10 -0.529031 1.755489 -0.000042
 C11 -1.313571 0.682604 -0.000040
 N12 1.664013 2.448484 -0.000008
 H13 1.325247 3.398029 -0.000028
 H14 2.657521 2.284065 0.000022
 O15 0.940374 -2.121943 0.000057
 H16 -4.175764 -0.907789 -0.000073
 H17 -2.124212 -2.421757 -0.000004
 O18 3.713689 -1.059392 0.000106
 H19 3.337699 -1.950160 0.000111

H20 4.672010 -1.147096 0.000084

Zero-point correction= 0.153605 (Hartree/Particle)
 Thermal correction to Energy= 0.165628
 Thermal correction to Enthalpy= 0.166572
 Thermal correction to Gibbs Free Energy= 0.115306
 Sum of electronic and zero-point Energies= -619.416104
 Sum of electronic and thermal Energies= -619.404082
 Sum of electronic and thermal Enthalpies= -619.403137
 Sum of electronic and thermal Free Energies= -619.454403

[G + H]⁺₁··W2

C1 -1.167446 1.504534 -0.000030
 C2 -1.528659 0.112278 0.000004
 H3 0.586274 2.565455 -0.000063
 C4 1.152777 0.562131 -0.000019
 H5 -0.808369 -2.993080 0.000069
 C6 -2.565198 -1.838568 0.000051
 N7 0.248276 1.609281 -0.000039
 N8 -2.756449 -0.523835 0.000023
 N9 -1.240348 -2.076961 0.000051
 N10 0.768011 -0.713133 0.000013
 C11 -0.551143 -0.867192 0.000022
 N12 2.452554 0.857417 -0.000032
 H13 3.155240 0.112950 -0.000016
 H14 2.780152 1.809983 -0.000052
 O15 -1.893912 2.470861 -0.000049
 H16 -3.338503 -2.588897 0.000071
 H17 -3.657653 -0.059258 0.000016
 O18 4.713737 -0.886050 0.000007
 H19 5.188943 -1.217100 0.769695
 H20 5.189017 -1.217028 -0.769666

Zero-point correction= 0.153326 (Hartree/Particle)
 Thermal correction to Energy= 0.165585
 Thermal correction to Enthalpy= 0.166529
 Thermal correction to Gibbs Free Energy= 0.114133
 Sum of electronic and zero-point Energies= -619.411991
 Sum of electronic and thermal Energies= -619.399732
 Sum of electronic and thermal Enthalpies= -619.398788
 Sum of electronic and thermal Free Energies= -619.451184

[G + H]⁺₂··W23

C1 -1.180980 1.315273 0.000000
 C2 -1.385006 -0.071952 0.000001
 C3 1.106320 0.991375 0.000005
 C4 -1.940867 -2.193967 -0.000002
 N5 0.047814 1.810980 0.000004
 N6 -2.461557 -0.939077 -0.000004
 N7 -0.614089 -2.211883 0.000003
 N8 0.981432 -0.367799 0.000007
 C9 -0.273274 -0.908180 0.000004
 N10 2.335781 1.514789 -0.000001
 H11 3.155687 0.920702 -0.000004
 H12 2.430578 2.518284 0.000007
 O13 -2.220936 2.131825 -0.000005
 H14 -2.564844 -3.075361 -0.000004
 H15 -3.441212 -0.690275 -0.000006
 H16 -1.914404 3.053142 -0.000006

H17 1.821468 -0.955814 0.000009
 O18 3.740339 -1.151483 -0.000008
 H19 4.187324 -1.528905 0.768316
 H20 4.187356 -1.528884 -0.768323

Zero-point correction= 0.154473 (Hartree/Particle)
 Thermal correction to Energy= 0.165973
 Thermal correction to Enthalpy= 0.166917
 Thermal correction to Gibbs Free Energy= 0.117167
 Sum of electronic and zero-point Energies= -619.417478
 Sum of electronic and thermal Energies= -619.405978
 Sum of electronic and thermal Enthalpies= -619.405034
 Sum of electronic and thermal Free Energies= -619.454784

[G + H]⁺₂··W39

C1 1.722313 0.554013 0.000002
 C2 1.041487 -0.672641 -0.000003
 C3 -0.295107 1.684129 -0.000008
 C4 0.186199 -2.693483 -0.000002
 N5 1.044404 1.691965 0.000002
 N6 1.363593 -2.017091 0.000006
 N7 -0.875585 -1.896738 -0.000016
 N8 -1.020397 0.534182 -0.000026
 C9 -0.347497 -0.652990 -0.000017
 N10 -0.936498 2.859508 -0.000006
 H11 -1.941371 2.930611 0.000041
 H12 -0.387521 3.705300 0.000025
 O13 3.043870 0.571973 0.000011
 H14 0.143007 -3.772454 0.000003
 H15 2.291044 -2.419192 0.000017
 H16 3.360438 1.489979 0.000017
 H17 -2.055340 0.492170 -0.000046
 O18 -3.585480 -0.368601 0.000073
 H19 -3.409301 -1.319001 0.000044
 H20 -4.541073 -0.251332 -0.000314

Zero-point correction= 0.153283 (Hartree/Particle)
 Thermal correction to Energy= 0.165304
 Thermal correction to Enthalpy= 0.166248
 Thermal correction to Gibbs Free Energy= 0.114846
 Sum of electronic and zero-point Energies= -619.415313
 Sum of electronic and thermal Energies= -619.403292
 Sum of electronic and thermal Enthalpies= -619.402348
 Sum of electronic and thermal Free Energies= -619.453750

[G + H]⁺₂··W6

C1 0.657775 -0.523318 -0.022498
 C2 -0.730921 -0.759102 -0.010664
 C3 0.255361 1.759321 -0.001511
 C4 -2.834248 -1.386477 0.008926
 N5 1.103909 0.733859 -0.021682
 N6 -1.562186 -1.863032 -0.008345
 N7 -2.894732 -0.060334 0.018778
 N8 -1.101629 1.594781 0.012252
 C9 -1.603357 0.318536 0.006663
 N10 0.755599 3.003817 0.002453
 H11 0.181719 3.830945 0.032832
 H12 1.758293 3.109512 0.011935
 O13 1.483772 -1.531776 -0.037002

H14 -3.694898 -2.038507 0.013741
 H15 -1.278076 -2.832945 -0.018795
 H16 2.449465 -1.264561 -0.024209
 H17 -1.744479 2.378392 0.027242
 O18 4.078460 -1.099415 0.056721
 H19 4.631019 -1.732462 0.529289
 H20 4.624700 -0.718223 -0.639488

Zero-point correction= 0.152884 (Hartree/Particle)
 Thermal correction to Energy= 0.165118
 Thermal correction to Enthalpy= 0.166062
 Thermal correction to Gibbs Free Energy= 0.113860
 Sum of electronic and zero-point Energies= -619.415415
 Sum of electronic and thermal Energies= -619.403182
 Sum of electronic and thermal Enthalpies= -619.402237
 Sum of electronic and thermal Free Energies= -619.454440

[G + H]⁺₂··W7

C1 -0.260197 -1.214342 0.000003
 C2 0.390247 0.025934 0.000003
 C3 -2.322715 -0.164509 -0.000003
 C4 1.600956 1.842134 0.000006
 N5 -1.588821 -1.277236 -0.000001
 N6 1.689543 0.492372 0.000006
 N7 0.348130 2.299299 0.000003
 N8 -1.758060 1.078304 -0.000002
 C9 -0.390405 1.180799 0.000001
 N10 -3.658135 -0.276333 -0.000007
 H11 -4.279132 0.516776 -0.000009
 H12 -4.057129 -1.202607 -0.000008
 O13 0.439898 -2.334223 0.000006
 H14 2.476744 2.473724 0.000007
 H15 2.564477 -0.053917 0.000004
 H16 -0.163426 -3.094934 0.000005
 H17 -2.313965 1.926393 -0.000002
 O18 4.190939 -0.755985 -0.000009
 H19 4.694892 -1.039424 0.771015
 H20 4.694940 -1.039289 -0.771051

Zero-point correction= 0.153008 (Hartree/Particle)
 Thermal correction to Energy= 0.165315
 Thermal correction to Enthalpy= 0.166259
 Thermal correction to Gibbs Free Energy= 0.114098
 Sum of electronic and zero-point Energies= -619.413709
 Sum of electronic and thermal Energies= -619.401402
 Sum of electronic and thermal Enthalpies= -619.400457
 Sum of electronic and thermal Free Energies= -619.452619

[G + H]⁺₂··W2

C1 0.234621 1.270824 0.000034
 C2 1.400795 0.490156 -0.000003
 C3 -1.077196 -0.637811 0.000058
 C4 3.343350 -0.529820 -0.000061
 N5 -0.957464 0.696841 0.000068
 N6 2.767328 0.700320 -0.000042
 N7 2.460404 -1.521386 -0.000038
 N8 0.023101 -1.456549 0.000027
 C9 1.270967 -0.892370 -0.000004
 N10 -2.292435 -1.178313 0.000084

H11 -2.428867 -2.177091 0.000045
 H12 -3.128037 -0.582987 0.000091
 O13 0.329708 2.589406 0.000033
 H14 4.414765 -0.664549 -0.000091
 H15 3.244113 1.591648 -0.000054
 H16 -0.559239 2.980230 0.000053
 H17 -0.059128 -2.466971 0.000028
 O18 -4.810120 0.125016 -0.000131
 H19 -5.341011 0.355888 0.769988
 H20 -5.341074 0.356192 -0.770116

Zero-point correction= 0.153136 (Hartree/Particle)
 Thermal correction to Energy= 0.165364
 Thermal correction to Enthalpy= 0.166308
 Thermal correction to Gibbs Free Energy= 0.114048
 Sum of electronic and zero-point Energies= -619.410617
 Sum of electronic and thermal Energies= -619.398389
 Sum of electronic and thermal Enthalpies= -619.397445
 Sum of electronic and thermal Free Energies= -619.449705

[G + H]⁺₃··W7

C1 0.106355 -1.169465 -0.001074
 C2 -0.403512 0.140234 -0.000833
 C3 2.236874 -0.275382 0.000555
 C4 -1.499693 2.045830 -0.001030
 N5 1.402568 -1.356654 -0.000484
 N6 -1.657988 0.731384 -0.001664
 N7 -0.184411 2.343594 0.000191
 N8 1.856318 1.019459 0.001013
 C9 0.548108 1.160120 0.000240
 N10 3.551131 -0.540227 0.001212
 H11 4.214882 0.217329 0.001977
 H12 3.872634 -1.494299 0.000876
 O13 -0.733746 -2.207229 -0.001713
 H14 -2.297152 2.770984 -0.001494
 H15 -0.210702 -3.025234 -0.002116
 H16 0.209517 3.276096 0.000815
 H17 -2.557212 0.208164 -0.002767
 O18 -3.740616 -1.014902 0.002072
 H19 -4.703595 -1.036882 0.008014
 H20 -3.435592 -1.930023 0.002802

Zero-point correction= 0.153306 (Hartree/Particle)
 Thermal correction to Energy= 0.165285
 Thermal correction to Enthalpy= 0.166229
 Thermal correction to Gibbs Free Energy= 0.114856
 Sum of electronic and zero-point Energies= -619.414126
 Sum of electronic and thermal Energies= -619.402147
 Sum of electronic and thermal Enthalpies= -619.401203
 Sum of electronic and thermal Free Energies= -619.452576

[G + H]⁺₃··W9

C1 1.745892 -0.789798 -0.000002
 C2 0.355971 -1.002708 0.000000
 C3 1.326121 1.481854 0.000001
 C4 -1.755675 -1.649662 0.000005
 N5 2.205112 0.437067 -0.000001
 N6 -0.499912 -2.096839 0.000001
 N7 -1.759246 -0.311821 0.000006

N8 -0.019437 1.389215 0.000002
 C9 -0.442531 0.141096 0.000002
 N10 1.868095 2.709247 0.000001
 H11 1.271490 3.520362 0.000002
 H12 2.869046 2.816892 0.000000
 O13 2.566201 -1.837073 -0.000004
 H14 -2.636256 -2.271543 0.000007
 H15 3.484341 -1.522451 -0.000005
 H16 -2.616820 0.273505 0.000011
 H17 -0.227864 -3.071575 -0.000001
 O18 -4.178991 1.016552 -0.000005
 H19 -4.591294 1.423082 -0.771092
 H20 -4.591287 1.423116 0.771067

Zero-point correction= 0.153364 (Hartree/Particle)
 Thermal correction to Energy= 0.165378
 Thermal correction to Enthalpy= 0.166322
 Thermal correction to Gibbs Free Energy= 0.114838
 Sum of electronic and zero-point Energies= -619.413731
 Sum of electronic and thermal Energies= -619.401717
 Sum of electronic and thermal Enthalpies= -619.400773
 Sum of electronic and thermal Free Energies= -619.452257

[G + H]⁺_3^{··}W6

C1 0.681120 -0.527860 0.000352
 C2 -0.721192 -0.712029 0.000168
 C3 0.276319 1.753593 0.000077
 C4 -2.839348 -1.353070 -0.000195
 N5 1.146416 0.703985 0.000327
 N6 -1.586094 -1.797731 0.000067
 N7 -2.824945 -0.009174 -0.000273
 N8 -1.073583 1.681173 -0.000116
 C9 -1.503288 0.438389 -0.000062
 N10 0.824038 2.978817 0.000045
 H11 0.230858 3.792630 -0.000281
 H12 1.824897 3.082245 -0.000055
 O13 1.459063 -1.584444 0.000564
 H14 -3.723499 -1.969315 -0.000324
 H15 2.428501 -1.345521 0.000286
 H16 -3.643609 0.586950 -0.000476
 H17 -1.314967 -2.773423 0.000155
 O18 4.063788 -1.137004 -0.001295
 H19 4.504299 -0.281007 0.002504
 H20 4.748230 -1.814610 0.001648

Zero-point correction= 0.152954 (Hartree/Particle)
 Thermal correction to Energy= 0.165248
 Thermal correction to Enthalpy= 0.166192
 Thermal correction to Gibbs Free Energy= 0.113401
 Sum of electronic and zero-point Energies= -619.411537
 Sum of electronic and thermal Energies= -619.399242
 Sum of electronic and thermal Enthalpies= -619.398298
 Sum of electronic and thermal Free Energies= -619.451089

[G + H]⁺_3^{··}W2a

C1 -0.190024 1.284625 0.000003
 C2 -1.356644 0.494703 0.000002
 C3 1.056985 -0.666721 -0.000004
 C4 -3.350815 -0.464937 0.000002

N5 0.978849 0.700825 -0.000002
 N6 -2.728888 0.710398 0.000005
 N7 -2.433054 -1.446173 -0.000003
 N8 -0.003343 -1.514394 -0.000006
 C9 -1.153940 -0.885405 -0.000003
 N10 2.278522 -1.196852 -0.000006
 H11 2.367295 -2.200764 -0.000015
 H12 3.119684 -0.620222 0.000013
 O13 -0.305433 2.610430 0.000006
 H14 -4.419160 -0.607497 0.000004
 H15 0.581754 3.004356 0.000010
 H16 -2.634353 -2.438733 -0.000005
 H17 -3.192559 1.610603 0.000008
 O18 4.883754 0.066817 0.000002
 H19 5.436486 0.241753 0.769035
 H20 5.436325 0.242314 -0.769020

Zero-point correction= 0.153366 (Hartree/Particle)
 Thermal correction to Energy= 0.165545
 Thermal correction to Enthalpy= 0.166489
 Thermal correction to Gibbs Free Energy= 0.114236
 Sum of electronic and zero-point Energies= -619.404503
 Sum of electronic and thermal Energies= -619.392324
 Sum of electronic and thermal Enthalpies= -619.391380
 Sum of electronic and thermal Free Energies= -619.443633

[G + H]⁺_3^{··}W2b

C1 -1.026675 1.419776 -0.000049
 C2 -1.500376 0.093038 -0.000077
 C3 1.133876 0.578755 0.000256
 C4 -2.541897 -1.859368 -0.000096
 N5 0.261752 1.637809 0.000117
 N6 -2.734795 -0.543664 -0.000188
 N7 -1.221749 -2.108565 0.000072
 N8 0.779265 -0.729792 0.000268
 C9 -0.520849 -0.900266 0.000093
 N10 2.430916 0.880398 0.000412
 H11 3.153735 0.160684 0.000380
 H12 2.700426 1.851182 0.000652
 O13 -1.903681 2.420504 -0.000203
 H14 -3.319674 -2.605510 -0.000146
 H15 -1.423545 3.264081 -0.000177
 H16 -0.797311 -3.028051 0.000159
 H17 -3.640848 -0.091458 -0.000319
 O18 4.766718 -0.830380 -0.000384
 H19 5.276306 -1.105857 -0.769746
 H20 5.274414 -1.110977 0.768363

Zero-point correction= 0.153285 (Hartree/Particle)
 Thermal correction to Energy= 0.165517
 Thermal correction to Enthalpy= 0.166462
 Thermal correction to Gibbs Free Energy= 0.113933
 Sum of electronic and zero-point Energies= -619.404409
 Sum of electronic and thermal Energies= -619.392177
 Sum of electronic and thermal Enthalpies= -619.391233
 Sum of electronic and thermal Free Energies= -619.443761

[G + H]⁺_4^{··}W23

C1 -1.311726 1.401449 0.000016

C2 -1.435096 -0.023321 0.000010
 C3 1.163867 0.931291 -0.000028
 C4 -2.040768 -2.132143 -0.000007
 N5 0.099842 1.763272 -0.000003
 N6 -2.526355 -0.864942 0.000017
 N7 -0.713251 -2.172889 -0.000030
 N8 0.949206 -0.394601 -0.000037
 C9 -0.350017 -0.876740 -0.000018
 N10 2.413840 1.398566 -0.000035
 H11 3.188718 0.740875 -0.000024
 H12 2.608051 2.387408 -0.000042
 O13 -2.148339 2.265252 0.000033
 H14 -2.682971 -2.999641 -0.000007
 H15 -3.497871 -0.582968 0.000036
 H16 0.255457 2.765539 0.000010
 H17 1.753241 -1.027842 -0.000073
 O18 3.698810 -1.251270 0.000057
 H19 4.125498 -1.652140 0.768569
 H20 4.125565 -1.652150 -0.768414

Zero-point correction= 0.154216 (Hartree/Particle)
 Thermal correction to Energy= 0.165895
 Thermal correction to Enthalpy= 0.166839
 Thermal correction to Gibbs Free Energy= 0.116681
 Sum of electronic and zero-point Energies= -619.415283
 Sum of electronic and thermal Energies= -619.403603
 Sum of electronic and thermal Enthalpies= -619.402659
 Sum of electronic and thermal Free Energies= -619.452817

[G + H]⁺_4^{...}W12

C1 0.001105 1.305885 0.000017
 C2 -1.236446 0.584235 0.000002
 H3 2.040598 0.792433 0.000017
 C4 1.049693 -0.976791 0.000015
 H5 -0.250708 -2.582261 0.000004
 C6 -3.307488 -0.143696 -0.000021
 N7 1.108551 0.370113 0.000020
 N8 -2.554689 0.985729 -0.000009
 N9 -2.571099 -1.249318 -0.000018
 N10 -0.157481 -1.573884 0.000005
 C11 -1.306369 -0.792680 -0.000004
 N12 2.177260 -1.688789 0.000026
 H13 2.167411 -2.696825 0.000011
 H14 3.070259 -1.200602 0.000032
 O15 0.213717 2.490677 0.000026
 H16 -4.386572 -0.123184 -0.000032
 H17 -2.887398 1.941089 -0.000009
 O18 4.032298 0.555545 -0.000061
 H19 4.528674 0.865395 0.768512
 H20 4.528858 0.865501 -0.768471

Zero-point correction= 0.154216 (Hartree/Particle)
 Thermal correction to Energy= 0.165921
 Thermal correction to Enthalpy= 0.166866
 Thermal correction to Gibbs Free Energy= 0.116663
 Sum of electronic and zero-point Energies= -619.414712
 Sum of electronic and thermal Energies= -619.403006
 Sum of electronic and thermal Enthalpies= -619.402062
 Sum of electronic and thermal Free Energies= -619.452265

[G + H]⁺_4^{...}W39

C1 1.870362 0.524031 0.000000
 C2 1.081581 -0.670179 0.000001
 H3 1.488851 2.564674 -0.000002
 C4 -0.364758 1.690847 0.000001
 C5 0.239428 -2.696843 0.000000
 N6 0.987345 1.682926 0.000000
 N7 1.408003 -2.009137 0.000000
 N8 -0.823262 -1.898927 0.000001
 N9 -1.019650 0.525193 0.000002
 C10 -0.296601 -0.655211 0.000001
 N11 -1.037704 2.847309 0.000000
 H12 -2.046410 2.860491 -0.000004
 H13 -0.562802 3.736507 -0.000003
 O14 3.062061 0.680680 -0.000001
 H15 0.200408 -3.775388 -0.000001
 H16 2.342788 -2.396245 -0.000001
 H17 -2.053864 0.439511 0.000004
 O18 -3.497440 -0.514930 -0.000007
 H19 -3.209204 -1.439209 -0.000004
 H20 -4.459938 -0.503759 0.000039

Zero-point correction= 0.152932 (Hartree/Particle)
 Thermal correction to Energy= 0.165146
 Thermal correction to Enthalpy= 0.166091
 Thermal correction to Gibbs Free Energy= 0.114398
 Sum of electronic and zero-point Energies= -619.412799
 Sum of electronic and thermal Energies= -619.400585
 Sum of electronic and thermal Enthalpies= -619.399640
 Sum of electronic and thermal Free Energies= -619.451333

[G + H]⁺_4^{...}W16

C1 -0.376410 -1.054636 0.000000
 C2 1.000079 -0.666723 -0.000001
 H3 -2.232437 -0.117767 -0.000003
 C4 -0.832960 1.401284 0.000000
 C5 3.186163 -0.468964 0.000000
 N6 -1.222735 0.117675 -0.000001
 N7 2.179484 -1.379496 0.000000
 N8 2.743929 0.783742 0.000000
 N9 0.483300 1.688408 0.000000
 C10 1.406255 0.651393 0.000000
 N11 -1.741726 2.383151 0.000000
 H12 -1.475823 3.355797 0.000002
 H13 -2.727973 2.171657 0.000004
 O14 -0.874173 -2.155613 0.000002
 H15 4.227311 -0.753565 0.000000
 H16 2.268098 -2.387229 0.000000
 H17 0.820727 2.643446 0.000002
 O18 -3.665869 -1.104035 0.000001
 H19 -4.627298 -1.154030 -0.000020
 H20 -3.326789 -2.009609 0.000007

Zero-point correction= 0.152897 (Hartree/Particle)
 Thermal correction to Energy= 0.165224
 Thermal correction to Enthalpy= 0.166168
 Thermal correction to Gibbs Free Energy= 0.114102

Sum of electronic and zero-point Energies=	-619.411795
Sum of electronic and thermal Energies=	-619.399468
Sum of electronic and thermal Enthalpies=	-619.398524
Sum of electronic and thermal Free Energies=	-619.450590

[G + H]₄⁺W67

C1	-0.154880	-1.185175	0.000000
C2	-0.514749	0.193228	0.000000
H3	1.614557	-2.275115	0.000000
C4	2.213858	-0.320387	0.000000
C5	-1.459438	2.160291	0.000000
N6	1.298750	-1.310998	0.000000
N7	-1.729278	0.837591	0.000001
N8	-0.150282	2.428323	0.000000
N9	1.782280	0.950392	0.000000
C10	0.416666	1.215959	0.000000
N11	3.522406	-0.598754	0.000000
H12	4.218147	0.131877	-0.000001
H13	3.858137	-1.549760	-0.000001
O14	-0.826334	-2.188437	0.000001
H15	-2.233444	2.912333	0.000000
H16	-2.636730	0.344235	0.000000
H17	2.429290	1.730381	0.000000
O18	-3.631843	-1.125122	-0.000003
H19	-3.101129	-1.933296	0.000000
H20	-4.559290	-1.381540	0.000011

Zero-point correction=	0.153059 (Hartree/Particle)
Thermal correction to Energy=	0.165202
Thermal correction to Enthalpy=	0.166146
Thermal correction to Gibbs Free Energy=	0.115105
Sum of electronic and zero-point Energies=	-619.409488
Sum of electronic and thermal Energies=	-619.397344
Sum of electronic and thermal Enthalpies=	-619.396400
Sum of electronic and thermal Free Energies=	-619.447441

Cartesian coordinates for the structures of monohydrated deprotonated guanine tautomers in Fig. S4, optimized at B3LYP/6-311++G**

[G – H]⁻_1^{··}W67

C1 0.116313 -1.147171 -0.024847
 C2 0.434127 0.250145 -0.004315
 C3 -2.096408 -0.393904 0.026741
 C4 1.306928 2.260783 -0.018459
 N5 -1.218864 -1.412948 -0.003637
 N6 1.634471 0.940247 -0.025194
 N7 0.005327 2.486592 0.001076
 N8 -1.883023 0.922563 0.024509
 C9 -0.563418 1.223265 0.010311
 N10 -3.444132 -0.788806 0.099814
 H11 -4.073250 -0.085118 -0.259945
 H12 -3.593441 -1.712371 -0.280536
 O13 0.992660 -2.064342 -0.065027
 H14 2.063536 3.033202 -0.027600
 H15 2.550843 0.494514 -0.021420
 O16 3.483316 -1.263135 -0.023739
 H17 3.860070 -1.663295 0.764232
 H18 2.542731 -1.639350 -0.077162

Zero-point correction= 0.128284 (Hartree/Particle)
 Thermal correction to Energy= 0.138677
 Thermal correction to Enthalpy= 0.139621
 Thermal correction to Gibbs Free Energy= 0.092260
 Sum of electronic and zero-point Energies= -618.525407
 Sum of electronic and thermal Energies= -618.515014
 Sum of electronic and thermal Enthalpies= -618.514070
 Sum of electronic and thermal Free Energies= -618.561431

[G – H]⁻_1^{··}W16

C1 0.548998 -0.852766 -0.001102
 C2 -0.865635 -0.621511 -0.012089
 C3 0.659539 1.496810 -0.014776
 C4 -3.062710 -0.700277 0.008149
 N5 1.286636 0.305498 -0.007470
 N6 -1.945175 -1.485191 -0.001012
 N7 -2.793235 0.589591 0.005720
 N8 -0.645017 1.777532 -0.004737
 C9 -1.406669 0.658716 -0.006475
 N10 1.513268 2.609124 -0.069890
 H11 1.079027 3.449450 0.283855
 H12 2.429677 2.422874 0.310507
 O13 1.054639 -2.002982 0.016948
 H14 -4.057000 -1.124707 0.014572
 H15 -1.884640 -2.490485 -0.000331
 O16 3.809387 -1.297245 -0.003007
 H17 3.020103 -1.871719 0.017986
 H18 3.344148 -0.445310 -0.038630

Zero-point correction= 0.128022 (Hartree/Particle)
 Thermal correction to Energy= 0.139000
 Thermal correction to Enthalpy= 0.139944
 Thermal correction to Gibbs Free Energy= 0.090382
 Sum of electronic and zero-point Energies= -618.522383
 Sum of electronic and thermal Energies= -618.511405

Sum of electronic and thermal Enthalpies= -618.510461
 Sum of electronic and thermal Free Energies= -618.560023

[G – H]⁻_1^{··}W39

C1 1.913373 0.167197 0.005170
 C2 0.852667 -0.809324 -0.012071
 C3 0.127541 1.699072 -0.022064
 C4 -0.438000 -2.594201 0.000687
 N5 1.444959 1.461477 0.000015
 N6 0.864878 -2.192349 0.000919
 N7 -1.287173 -1.583580 -0.010250
 N8 -0.903267 0.840095 -0.024178
 C9 -0.485706 -0.449498 -0.018128
 N10 -0.225823 3.055327 -0.080415
 H11 -1.145275 3.246287 0.291079
 H12 0.502528 3.656964 0.275489
 O13 3.120900 -0.143328 0.029423
 H14 -0.717583 -3.637940 0.007136
 H15 1.695292 -2.762341 0.009539
 O16 -3.758253 0.185544 0.029349
 H17 -3.372100 -0.702708 0.028622
 H18 -2.938304 0.715740 -0.006258

Zero-point correction= 0.128075 (Hartree/Particle)
 Thermal correction to Energy= 0.139045
 Thermal correction to Enthalpy= 0.139989
 Thermal correction to Gibbs Free Energy= 0.090610
 Sum of electronic and zero-point Energies= -618.519724
 Sum of electronic and thermal Energies= -618.508754
 Sum of electronic and thermal Enthalpies= -618.507810
 Sum of electronic and thermal Free Energies= -618.557189

[G – H]⁻_1^{··}W23

C1 1.222178 1.415119 0.041988
 C2 1.308980 -0.023566 -0.000696
 C3 -1.091339 1.008389 -0.078503
 C4 1.879162 -2.149226 -0.018837
 N5 -0.073823 1.874752 -0.006038
 N6 2.390592 -0.884516 0.026618
 N7 0.560962 -2.172558 -0.072780
 N8 -1.072242 -0.337571 -0.096759
 C9 0.188455 -0.837977 -0.060499
 N10 -2.359569 1.586247 -0.181362
 H11 -3.122852 0.981967 0.095335
 H12 -2.392121 2.525745 0.183846
 O13 2.225935 2.151866 0.117324
 H14 2.513894 -3.024134 -0.012014
 H15 3.354922 -0.597894 0.074808
 O16 -3.609933 -1.377429 0.262535
 H17 -2.646811 -1.135529 0.160560
 H18 -3.801108 -1.886569 -0.529869

Zero-point correction= 0.127559 (Hartree/Particle)
 Thermal correction to Energy= 0.138635
 Thermal correction to Enthalpy= 0.139579
 Thermal correction to Gibbs Free Energy= 0.090022
 Sum of electronic and zero-point Energies= -618.519310
 Sum of electronic and thermal Energies= -618.508234
 Sum of electronic and thermal Enthalpies= -618.507290

Sum of electronic and thermal Free Energies= -618.556848

[G - H]_2^W67

C1 -0.196562 -1.127448 -0.005115
 C2 -0.526128 0.254620 0.009112
 H3 1.526440 -2.252225 -0.135983
 C4 2.144462 -0.278365 -0.006600
 C5 -1.401717 2.175612 -0.000630
 N6 1.220458 -1.297631 -0.009054
 N7 -1.747861 0.884133 0.010329
 N8 -0.073826 2.467061 -0.008939
 N9 1.847199 0.978124 0.007498
 C10 0.491341 1.244008 -0.004834
 N11 3.491219 -0.695687 -0.066041
 H12 4.088031 0.117287 0.027781
 H13 3.726603 -1.386509 0.638325
 O14 -0.901885 -2.144546 -0.023152
 H15 -2.148274 2.961552 -0.002054
 O16 -3.742200 -1.255577 0.018623
 H17 -3.312096 -0.377041 0.019322
 H18 -2.956716 -1.824656 0.000682

Zero-point correction= 0.128566 (Hartree/Particle)
 Thermal correction to Energy= 0.139318
 Thermal correction to Enthalpy= 0.140262
 Thermal correction to Gibbs Free Energy= 0.091568
 Sum of electronic and zero-point Energies= -618.522094
 Sum of electronic and thermal Energies= -618.511342
 Sum of electronic and thermal Enthalpies= -618.510397
 Sum of electronic and thermal Free Energies= -618.559092

[G - H]_2^W39

C1 1.849060 -0.578661 0.009720
 C2 0.537015 -1.136135 0.012967
 H3 2.660530 1.318355 -0.120231
 C4 0.615165 1.600332 -0.015161
 C5 -1.210834 -2.315792 -0.003672
 N6 1.769139 0.857853 -0.000124
 N7 0.115856 -2.443756 0.018323
 N8 -1.715365 -1.048587 -0.023765
 N9 -0.574171 1.092559 -0.010784
 C10 -0.599851 -0.290741 -0.015540
 N11 0.798630 2.996109 -0.081217
 H12 -0.098853 3.456177 0.008888
 H13 1.446804 3.348465 0.614293
 O14 2.967725 -1.089395 0.005430
 H15 -1.869094 -3.176984 -0.004801
 O16 -3.699476 1.026965 0.024139
 H17 -3.290427 0.134960 0.006315
 H18 -2.896902 1.565201 0.012075

Zero-point correction= 0.128028 (Hartree/Particle)
 Thermal correction to Energy= 0.139058
 Thermal correction to Enthalpy= 0.140002
 Thermal correction to Gibbs Free Energy= 0.090354
 Sum of electronic and zero-point Energies= -618.519831
 Sum of electronic and thermal Energies= -618.508801
 Sum of electronic and thermal Enthalpies= -618.507857
 Sum of electronic and thermal Free Energies= -618.557505

[G - H]_2^W23

C1 1.355169 1.322866 0.035654
 C2 1.431939 -0.098744 0.016083
 H3 -0.145606 2.739821 -0.093161
 C4 -1.116973 0.917759 -0.057166
 C5 1.939566 -2.143539 -0.006290
 N6 -0.023056 1.741292 0.000907
 N7 2.516868 -0.941132 0.043853
 N8 0.577024 -2.189281 -0.065662
 N9 -1.035399 -0.377225 -0.079319
 C10 0.252029 -0.884708 -0.054453
 N11 -2.363632 1.555786 -0.136029
 H12 -3.120235 0.886347 -0.024418
 H13 -2.464206 2.328601 0.510460
 O14 2.214840 2.202761 0.070353
 H15 2.526115 -3.055938 0.000234
 O16 -3.628256 -1.313070 0.057135
 H17 -2.647022 -1.180483 -0.037405
 H18 -3.714735 -2.043761 0.675174

Zero-point correction= 0.127753 (Hartree/Particle)
 Thermal correction to Energy= 0.138777
 Thermal correction to Enthalpy= 0.139721
 Thermal correction to Gibbs Free Energy= 0.090406
 Sum of electronic and zero-point Energies= -618.517923
 Sum of electronic and thermal Energies= -618.506899
 Sum of electronic and thermal Enthalpies= -618.505955
 Sum of electronic and thermal Free Energies= -618.555269

[G - H]_2^W16

C1 0.486995 -0.896919 0.051406
 C2 -0.918106 -0.740285 0.021171
 H3 2.158764 0.316387 -0.035380
 C4 0.511463 1.579916 0.002592
 C5 -3.015977 -0.892988 -0.027926
 N6 1.146116 0.362164 0.031303
 N7 -1.931386 -1.668854 0.017802
 N8 -2.832097 0.458643 -0.054004
 N9 -0.771237 1.740734 -0.015203
 C10 -1.491602 0.563572 -0.024404
 N11 1.367942 2.696830 -0.058138
 H12 0.826333 3.540727 0.079468
 H13 2.142722 2.651646 0.593587
 O14 1.194867 -1.927122 0.085711
 H15 -4.014652 -1.316762 -0.043598
 O16 3.757632 -1.181459 -0.012703
 H17 2.859101 -1.606307 0.068879
 H18 4.115739 -1.523434 -0.836377

Zero-point correction= 0.128056 (Hartree/Particle)
 Thermal correction to Energy= 0.138884
 Thermal correction to Enthalpy= 0.139828
 Thermal correction to Gibbs Free Energy= 0.091058
 Sum of electronic and zero-point Energies= -618.517425
 Sum of electronic and thermal Energies= -618.506597
 Sum of electronic and thermal Enthalpies= -618.505653
 Sum of electronic and thermal Free Energies= -618.554423

[G - H]_2W2**

C1 0.430086 1.457036 0.187240
 C2 1.419304 0.459194 -0.052725
 H3 -1.601752 1.476786 0.589807
 C4 -1.051034 -0.521322 0.552464
 C5 3.123573 -0.698743 -0.488341
 N6 -0.829583 0.831277 0.494349
 N7 2.745058 0.578947 -0.382331
 N8 2.183460 -1.657804 -0.262343
 N9 -0.158342 -1.424727 0.338171
 C10 1.090504 -0.922921 0.015183
 N11 -2.398552 -0.901674 0.827186
 H12 -2.415114 -1.913336 0.912900
 H13 -2.739198 -0.493198 1.694143
 O14 0.467917 2.686723 0.169053
 H15 4.142652 -0.968127 -0.744554
 O16 -4.318306 -0.013649 -1.209945
 H17 -3.775906 0.240767 -1.962299
 H18 -3.676459 -0.349084 -0.551025

Zero-point correction= 0.127388 (Hartree/Particle)
 Thermal correction to Energy= 0.138753
 Thermal correction to Enthalpy= 0.139697
 Thermal correction to Gibbs Free Energy= 0.088334
 Sum of electronic and zero-point Energies= -618.510689
 Sum of electronic and thermal Energies= -618.499325
 Sum of electronic and thermal Enthalpies= -618.498380
 Sum of electronic and thermal Free Energies= -618.549744

[G - H]_3W67**

C1 -0.015702 -1.103865 -0.046347
 C2 -0.477156 0.217025 -0.039529
 C3 2.126889 -0.286921 0.003480
 C4 -1.438952 2.107736 -0.018890
 N5 1.291107 -1.349443 -0.023984
 N6 -1.733063 0.796228 -0.050785
 N7 -0.136240 2.454458 0.013217
 N8 1.828427 1.003605 0.025613
 C9 0.495974 1.247984 -0.000644
 N10 3.493392 -0.617956 -0.028164
 H11 4.072551 0.113759 0.358664
 H12 3.679444 -1.533332 0.356019
 O13 -0.823942 -2.187053 -0.067383
 H14 -2.223462 2.856576 -0.020255
 H15 -1.766646 -1.909395 -0.075321
 O16 -3.464343 -1.198289 0.013762
 H17 -2.976445 -0.307519 -0.031540
 H18 -3.830837 -1.237350 0.901711

Zero-point correction= 0.128633 (Hartree/Particle)
 Thermal correction to Energy= 0.138836
 Thermal correction to Enthalpy= 0.139780
 Thermal correction to Gibbs Free Energy= 0.092849
 Sum of electronic and zero-point Energies= -618.521157
 Sum of electronic and thermal Energies= -618.510954
 Sum of electronic and thermal Enthalpies= -618.510010
 Sum of electronic and thermal Free Energies= -618.556941

[G - H]_3W39**

C1 1.784977 -0.106267 0.001074
 C2 0.688919 -0.958976 -0.012286
 C3 0.364542 1.679881 -0.020455
 C4 -0.770681 -2.469067 0.000667
 N5 1.635235 1.210445 -0.003100
 N6 0.561232 -2.330349 -0.000003
 N7 -1.528102 -1.337488 -0.008407
 N8 -0.769925 0.990461 -0.019871
 C9 -0.590785 -0.355456 -0.017208
 N10 0.258076 3.076988 -0.079631
 H11 -0.624659 3.418036 0.272953
 H12 1.063964 3.547290 0.306116
 O13 3.059844 -0.590699 0.026714
 H14 -1.237363 -3.447705 0.007976
 H15 2.970653 -1.554501 0.031004
 O16 -3.783994 0.502421 0.027372
 H17 -3.322748 -0.358595 0.023569
 H18 -3.014084 1.090617 -0.007963

Zero-point correction= 0.128573 (Hartree/Particle)
 Thermal correction to Energy= 0.139390
 Thermal correction to Enthalpy= 0.140334
 Thermal correction to Gibbs Free Energy= 0.091251
 Sum of electronic and zero-point Energies= -618.518601
 Sum of electronic and thermal Energies= -618.507783
 Sum of electronic and thermal Enthalpies= -618.506839
 Sum of electronic and thermal Free Energies= -618.555923

[G - H]_3W23**

C1 1.215102 1.236128 0.042823
 C2 1.333381 -0.145910 -0.007129
 C3 -1.053446 1.031375 -0.094584
 C4 1.802169 -2.190919 -0.017639
 N5 0.032552 1.834130 0.000032
 N6 2.413332 -0.998824 0.040615
 N7 0.442695 -2.213201 -0.097197
 N8 -1.086398 -0.299043 -0.139500
 C9 0.134284 -0.895300 -0.092238
 N10 -2.277785 1.696971 -0.187389
 H11 -3.074995 1.135951 0.085547
 H12 -2.255535 2.623974 0.209764
 O13 2.315536 2.035985 0.148085
 H14 2.370250 -3.114995 -0.002369
 H15 3.071343 1.431517 0.171738
 O16 -3.688047 -1.216342 0.162269
 H17 -2.728207 -1.025127 -0.020247
 H18 -3.662486 -1.960931 0.769421

Zero-point correction= 0.128109 (Hartree/Particle)
 Thermal correction to Energy= 0.139038
 Thermal correction to Enthalpy= 0.139982
 Thermal correction to Gibbs Free Energy= 0.090655
 Sum of electronic and zero-point Energies= -618.516908
 Sum of electronic and thermal Energies= -618.505980
 Sum of electronic and thermal Enthalpies= -618.505036
 Sum of electronic and thermal Free Energies= -618.554363

[G - H]_3W12**

C1 0.138029 -1.043328 -0.114902

C2 -1.151727 -0.549213 -0.034847
 C3 0.929846 1.111549 -0.096617
 C4 -3.190692 -0.091496 0.122312
 N5 1.186277 -0.226706 -0.150741
 N6 -2.384080 -1.159202 0.027685
 N7 -2.624594 1.145570 0.131358
 N8 -0.245234 1.712144 0.001797
 C9 -1.303382 0.862200 0.029890
 N10 2.062183 1.926256 -0.192937
 H11 1.904454 2.853081 0.173487
 H12 2.922544 1.489909 0.113041
 O13 0.394848 -2.383201 -0.147268
 H14 -4.267447 -0.207277 0.189565
 H15 -0.471824 -2.812645 -0.107490
 O16 3.917717 -0.719404 0.214209
 H17 3.967510 -1.345895 0.941372
 H18 2.949935 -0.681038 -0.000652

Zero-point correction= 0.128037 (Hartree/Particle)
 Thermal correction to Energy= 0.139006
 Thermal correction to Enthalpy= 0.139950
 Thermal correction to Gibbs Free Energy= 0.090653
 Sum of electronic and zero-point Energies= -618.514846
 Sum of electronic and thermal Energies= -618.503877
 Sum of electronic and thermal Enthalpies= -618.502933
 Sum of electronic and thermal Free Energies= -618.552229

[G - H]_4^W67

C1 -0.179057 -1.160005 0.000011
 C2 -0.466258 0.244102 0.000007
 H3 1.491434 -2.347245 0.000007
 C4 2.252866 -0.433977 -0.000005
 H5 0.529392 3.257433 -0.000010
 C6 -1.347780 2.195624 0.000007
 N7 1.197654 -1.380640 0.000005
 N8 -1.672284 0.932344 0.000013
 N9 0.027280 2.384792 -0.000002
 N10 1.927730 0.898330 -0.000009
 C11 0.621563 1.133948 -0.000002
 N12 3.453878 -0.931320 -0.000009
 H13 4.108028 -0.151517 -0.000016
 O14 -0.966772 -2.117672 0.000020
 H15 -2.039646 3.024880 0.000009
 O16 -3.738215 -1.240403 -0.000025
 H17 -3.354056 -0.348409 0.000005
 H18 -2.923051 -1.773236 -0.000044

Zero-point correction= 0.128024 (Hartree/Particle)
 Thermal correction to Energy= 0.138834
 Thermal correction to Enthalpy= 0.139779
 Thermal correction to Gibbs Free Energy= 0.090849
 Sum of electronic and zero-point Energies= -618.517992
 Sum of electronic and thermal Energies= -618.507182
 Sum of electronic and thermal Enthalpies= -618.506238
 Sum of electronic and thermal Free Energies= -618.555167

[G - H]_4^W2

C1 -0.193014 1.402287 -0.042631
 C2 -1.352455 0.554103 0.006901

H3 1.844056 1.145426 -0.138924
 C4 1.106343 -0.777896 -0.078229
 H5 -2.635464 -2.347144 0.058193
 C6 -3.311627 -0.294760 0.079314
 N7 0.979376 0.623436 -0.081827
 N8 -2.704900 0.858845 0.055176
 N9 -2.422688 -1.363040 0.049271
 N10 -0.018263 -1.542570 -0.035695
 C11 -1.147334 -0.833819 0.002102
 N12 2.330251 -1.246175 -0.114709
 H13 2.285603 -2.261095 -0.115630
 O14 -0.123163 2.630436 -0.053753
 H15 -4.380774 -0.446383 0.118173
 O16 4.693254 0.163116 0.078115
 H17 3.856724 -0.371051 -0.053320
 H18 4.711218 0.318870 1.026372

Zero-point correction= 0.126973 (Hartree/Particle)
 Thermal correction to Energy= 0.138182
 Thermal correction to Enthalpy= 0.139126
 Thermal correction to Gibbs Free Energy= 0.088032
 Sum of electronic and zero-point Energies= -618.517650
 Sum of electronic and thermal Energies= -618.506441
 Sum of electronic and thermal Enthalpies= -618.505497
 Sum of electronic and thermal Free Energies= -618.556591

[G - H]_4^W39

C1 1.925960 0.125554 0.024414
 C2 0.897064 -0.879724 0.001437
 H3 2.011317 2.178519 0.019652
 C4 -0.002643 1.791621 -0.024339
 H5 -2.189888 -1.622331 -0.050843
 C6 -0.277622 -2.664315 -0.018825
 N7 1.355804 1.410057 0.009732
 N8 0.965092 -2.265670 0.007111
 N9 -1.177864 -1.608231 -0.042927
 N10 -0.941522 0.792043 -0.041636
 C11 -0.434388 -0.448813 -0.028510
 N12 -0.237532 3.071132 -0.034299
 H13 -1.245693 3.206272 -0.068450
 O14 3.149369 -0.009277 0.053636
 H15 -0.609512 -3.692477 -0.024163
 O16 -3.609456 0.190502 -0.008116
 H17 -3.983791 0.534535 0.807556
 H18 -2.699814 0.604422 -0.058850

Zero-point correction= 0.127573 (Hartree/Particle)
 Thermal correction to Energy= 0.138393
 Thermal correction to Enthalpy= 0.139338
 Thermal correction to Gibbs Free Energy= 0.090460
 Sum of electronic and zero-point Energies= -618.517216
 Sum of electronic and thermal Energies= -618.506395
 Sum of electronic and thermal Enthalpies= -618.505451
 Sum of electronic and thermal Free Energies= -618.554329

[G - H]_4^W6

C1 -0.749801 -0.507335 -0.112665
 C2 0.645643 -0.808007 -0.040838
 H3 -1.931955 1.172858 -0.141931

C4 -0.017776 1.917901 -0.011004
 H5 3.657571 0.174391 0.152462
 C6 2.584277 -1.699447 0.048011
 N7 -0.969174 0.868153 -0.091569
 N8 1.323904 -2.019070 -0.030546
 N9 2.784475 -0.323175 0.091492
 N10 1.309880 1.583952 0.055122
 C11 1.539310 0.276516 0.035513
 N12 -0.508702 3.121393 -0.007264
 H13 0.273526 3.769937 0.052599
 O14 -1.704577 -1.301365 -0.185510
 H15 3.411312 -2.394337 0.078224
 O16 -4.426788 -0.965121 0.098661
 H17 -4.484220 -1.227715 1.021234
 H18 -3.467910 -1.059790 -0.102548

Zero-point correction= 0.126730 (Hartree/Particle)
 Thermal correction to Energy= 0.138272
 Thermal correction to Enthalpy= 0.139216
 Thermal correction to Gibbs Free Energy= 0.086062
 Sum of electronic and zero-point Energies= -618.512873
 Sum of electronic and thermal Energies= -618.501331
 Sum of electronic and thermal Enthalpies= -618.500387
 Sum of electronic and thermal Free Energies= -618.553541

[G - H]_5^{W67}

C1 -0.141038 -1.179678 -0.013131
 C2 -0.475891 0.235777 -0.013701
 C3 2.099174 -0.435510 -0.012155
 H4 0.450593 3.278462 0.006843
 C5 -1.398631 2.175346 0.000748
 N6 1.221203 -1.432407 -0.010863
 N7 -1.696689 0.903178 -0.010343
 N8 -0.031687 2.394718 0.007681
 N9 1.888187 0.896987 0.000914
 C10 0.572225 1.151961 -0.002543
 N11 3.448423 -0.816280 -0.063056
 H12 4.071521 -0.128942 0.335809
 H13 3.592735 -1.757829 0.271841
 O14 -0.974564 -2.104296 -0.008094
 H15 -2.107267 2.990780 0.004827
 O16 -3.713503 -1.329872 0.024206
 H17 -3.387258 -0.416669 0.012163
 H18 -2.856889 -1.803201 0.013989

Zero-point correction= 0.128137 (Hartree/Particle)
 Thermal correction to Energy= 0.138942
 Thermal correction to Enthalpy= 0.139886
 Thermal correction to Gibbs Free Energy= 0.091157
 Sum of electronic and zero-point Energies= -618.519335
 Sum of electronic and thermal Energies= -618.508530
 Sum of electronic and thermal Enthalpies= -618.507586
 Sum of electronic and thermal Free Energies= -618.556315

[G - H]_5^{W16}

C1 0.540887 -0.913812 -0.008073
 C2 -0.895394 -0.703107 -0.008514
 C3 0.680045 1.454742 -0.017853
 H4 -3.374902 1.287547 0.008309

C5 -3.032171 -0.842998 0.009194
 N6 1.281032 0.267102 -0.016090
 N7 -1.963274 -1.592295 -0.000277
 N8 -2.733184 0.511727 0.010518
 N9 -0.634010 1.742538 -0.002107
 C10 -1.356746 0.611072 -0.001895
 N11 1.528537 2.568903 -0.073282
 H12 1.108072 3.405736 0.304088
 H13 2.455974 2.375203 0.275217
 O14 1.095541 -2.025959 0.004099
 H15 -4.053290 -1.197359 0.015603
 O16 3.840929 -1.192003 0.012211
 H17 3.276977 -0.399174 -0.028002
 H18 3.121971 -1.849471 0.025826

Zero-point correction= 0.127632 (Hartree/Particle)
 Thermal correction to Energy= 0.138710
 Thermal correction to Enthalpy= 0.139654
 Thermal correction to Gibbs Free Energy= 0.089890
 Sum of electronic and zero-point Energies= -618.518780
 Sum of electronic and thermal Energies= -618.507702
 Sum of electronic and thermal Enthalpies= -618.506758
 Sum of electronic and thermal Free Energies= -618.556522

[G - H]_5^{W39}

C1 1.873563 0.487012 -0.048282
 C2 1.048828 -0.715936 -0.005185
 C3 -0.188736 1.656596 0.023816
 H4 -1.844556 -2.037891 0.104517
 C5 0.225740 -2.694935 0.046761
 N6 1.131262 1.673568 -0.020555
 N7 1.372046 -2.068157 -0.004816
 N8 -0.855676 -1.829796 0.084120
 N9 -1.027999 0.596630 0.064453
 C10 -0.330006 -0.558233 0.048697
 N11 -0.825774 2.909912 -0.005288
 H12 -1.714290 2.917636 0.476305
 H13 -0.199923 3.647570 0.285800
 O14 3.106862 0.498099 -0.097257
 H15 0.092707 -3.767392 0.062063
 O16 -3.606079 -0.348239 -0.056459
 H17 -2.748779 0.157729 0.019685
 H18 -3.924773 -0.138649 -0.938889

Zero-point correction= 0.127550 (Hartree/Particle)
 Thermal correction to Energy= 0.138509
 Thermal correction to Enthalpy= 0.139453
 Thermal correction to Gibbs Free Energy= 0.090270
 Sum of electronic and zero-point Energies= -618.515163
 Sum of electronic and thermal Energies= -618.504204
 Sum of electronic and thermal Enthalpies= -618.503260
 Sum of electronic and thermal Free Energies= -618.552443

[G - H]_6^{W39}

C1 1.761807 -0.309668 0.000808
 C2 0.598388 -1.066735 -0.007771
 C3 0.513235 1.621268 -0.019286
 C4 -1.029561 -2.397417 0.003297
 N5 1.726400 1.024885 -0.004870

N6 0.303928 -2.413422 0.003034
 N7 -1.657849 -1.186553 -0.005459
 N8 -0.673694 1.036614 -0.016902
 C9 -0.619035 -0.320670 -0.013331
 N10 0.539676 3.023784 -0.078543
 H11 -0.314514 3.439421 0.265205
 H12 1.373937 3.418093 0.331757
 O13 2.999138 -0.876416 0.019460
 H14 -1.605083 -3.316769 0.010011
 H15 3.612302 -0.128457 0.011743
 O16 -3.728572 0.841404 0.019714
 H17 -3.335931 -0.054314 0.019070
 H18 -2.913456 1.364291 -0.014301

Zero-point correction= 0.128307 (Hartree/Particle)
 Thermal correction to Energy= 0.139155
 Thermal correction to Enthalpy= 0.140099
 Thermal correction to Gibbs Free Energy= 0.091015
 Sum of electronic and zero-point Energies= -618.516281
 Sum of electronic and thermal Energies= -618.505433
 Sum of electronic and thermal Enthalpies= -618.504489
 Sum of electronic and thermal Free Energies= -618.553573

[G - H]_6··W67

C1 0.003608 -1.076311 -0.008631
 C2 -0.476112 0.224152 -0.012099
 C3 2.154791 -0.280908 -0.012640
 C4 -1.418099 2.109838 0.005270
 N5 1.308983 -1.339143 -0.010186
 N6 -1.725345 0.806017 -0.004811
 N7 -0.107116 2.457400 0.006520
 N8 1.847441 1.003949 -0.001429
 C9 0.514470 1.254570 -0.005112
 N10 3.519745 -0.613492 -0.068739
 H11 4.103581 0.136220 0.274797
 H12 3.723807 -1.508649 0.352403
 O13 -0.831714 -2.158703 -0.000351
 H14 -2.195679 2.865861 0.011888
 H15 -0.244595 -2.927233 -0.012570
 O16 -3.855012 -1.094720 0.014009
 H17 -3.253297 -0.312560 0.007172
 H18 -3.217912 -1.817414 0.006834

Zero-point correction= 0.127960 (Hartree/Particle)
 Thermal correction to Energy= 0.138923
 Thermal correction to Enthalpy= 0.139868
 Thermal correction to Gibbs Free Energy= 0.090470
 Sum of electronic and zero-point Energies= -618.516064
 Sum of electronic and thermal Energies= -618.505102
 Sum of electronic and thermal Enthalpies= -618.504157
 Sum of electronic and thermal Free Energies= -618.553555

[G - H]_6··W23

C1 1.235396 1.218145 0.039031
 C2 1.381846 -0.160825 0.003519
 C3 -1.050332 0.996295 -0.090560
 C4 1.824658 -2.213981 -0.017067
 N5 0.033341 1.798798 -0.012151
 N6 2.447582 -1.034124 0.035592

N7 0.461507 -2.227250 -0.079402
 N8 -1.062122 -0.331319 -0.105038
 C9 0.167097 -0.911945 -0.067109
 N10 -2.279920 1.650761 -0.207101
 H11 -3.077235 1.069450 0.021267
 H12 -2.288739 2.565965 0.217050
 O13 2.300633 2.061815 0.128473
 H14 2.384077 -3.143977 -0.011583
 H15 1.911568 2.947334 0.124108
 O16 -3.666141 -1.192856 0.271926
 H17 -2.688273 -1.045754 0.150710
 H18 -3.872036 -1.908894 -0.334931

Zero-point correction= 0.127815 (Hartree/Particle)
 Thermal correction to Energy= 0.138779
 Thermal correction to Enthalpy= 0.139723
 Thermal correction to Gibbs Free Energy= 0.090470
 Sum of electronic and zero-point Energies= -618.514295
 Sum of electronic and thermal Energies= -618.503331
 Sum of electronic and thermal Enthalpies= -618.502387
 Sum of electronic and thermal Free Energies= -618.551639

[G - H]_6··W16

C1 -0.354319 0.900423 0.077893
 C2 1.011586 0.666501 0.019506
 C3 -0.719238 -1.387334 0.025611
 C4 3.106883 0.560420 -0.057705
 N5 -1.221771 -0.128087 0.075691
 N6 2.130336 1.469591 0.003049
 N7 2.766400 -0.759430 -0.082552
 N8 0.545604 -1.748476 -0.022273
 C9 1.419434 -0.706275 -0.034061
 N10 -1.687364 -2.410845 -0.018318
 H11 -1.284394 -3.299944 0.244808
 H12 -2.520579 -2.190777 0.510556
 O13 -0.872029 2.150873 0.136406
 H14 4.149650 0.860596 -0.087034
 H15 -1.842522 2.076579 0.147250
 O16 -3.653073 1.086265 -0.092675
 H17 -2.882268 0.453556 -0.031790
 H18 -3.937585 1.041193 -1.010276

Zero-point correction= 0.128248 (Hartree/Particle)
 Thermal correction to Energy= 0.138899
 Thermal correction to Enthalpy= 0.139843
 Thermal correction to Gibbs Free Energy= 0.091593
 Sum of electronic and zero-point Energies= -618.511665
 Sum of electronic and thermal Energies= -618.501015
 Sum of electronic and thermal Enthalpies= -618.500070
 Sum of electronic and thermal Free Energies= -618.548320

**Cartesian coordinates for the structures in Fig. 2,
optimized at B3LYP/6-31+G***

[G + H]⁺

C1 0.250872 1.472780 0.000001
 C2 -0.788733 0.476071 0.000001
 H3 2.305537 1.461398 -0.000009
 C4 1.729149 -0.543420 0.000001
 H5 -1.805255 -2.551778 -0.000001
 C6 -2.696583 -0.643185 0.000000
 N7 1.515689 0.820513 0.000000
 N8 -2.168672 0.579119 0.000001
 N9 -1.691988 -1.542371 0.000000
 N10 0.739019 -1.432954 0.000002
 C11 -0.472575 -0.872848 0.000000
 N12 2.996835 -0.984803 -0.000011
 H13 3.155946 -1.984328 0.000019
 H14 3.800976 -0.373127 0.000045
 O15 0.139787 2.682848 -0.000001
 H16 -3.751047 -0.877737 -0.000001
 H17 -2.693412 1.449866 0.000001

Zero-point correction= 0.130035 (Hartree/Particle)
 Thermal correction to Energy= 0.138563
 Thermal correction to Enthalpy= 0.139507
 Thermal correction to Gibbs Free Energy= 0.096743
 Sum of electronic and zero-point Energies= -542.820021
 Sum of electronic and thermal Energies= -542.811492
 Sum of electronic and thermal Enthalpies= -542.810548
 Sum of electronic and thermal Free Energies= -542.853312

PC⁺

C1 -0.671958 1.499196 -0.175893
 C2 0.384800 0.554736 -0.467807
 H3 -2.662765 1.385320 0.317965
 C4 -2.034160 -0.582312 0.029939
 H5 1.476870 -2.421461 -0.895897
 C6 2.265742 -0.472708 -0.983120
 N7 -1.872930 0.786607 0.088187
 N8 1.695063 0.729510 -0.828824
 N9 1.315422 -1.419462 -0.848500
 N10 -1.043856 -1.424251 -0.277849
 C11 0.115643 -0.820340 -0.501014
 N12 -3.244494 -1.089655 0.290894
 H13 -3.358484 -2.095640 0.260805
 H14 -4.044950 -0.525997 0.543392
 O15 -0.607645 2.709405 -0.150520
 H16 3.298356 -0.650876 -1.244652
 H17 2.189357 1.618535 -0.839815
 O18 1.245738 -0.186766 1.788380
 O19 2.461505 -0.205208 1.546917

Zero-point correction= 0.135222 (Hartree/Particle)
 Thermal correction to Energy= 0.146893
 Thermal correction to Enthalpy= 0.147838
 Thermal correction to Gibbs Free Energy= 0.097534
 Sum of electronic and zero-point Energies= -693.084709
 Sum of electronic and thermal Energies= -693.073038
 Sum of electronic and thermal Enthalpies= -693.072094

Sum of electronic and thermal Free Energies= -693.122397

TS1a⁺

C1 -0.676386 1.501847 -0.137823
 C2 0.414851 0.568123 -0.378602
 H3 -2.681034 1.373162 0.294383
 C4 -2.024254 -0.585695 0.004538
 H5 1.531636 -2.416028 -0.702358
 C6 2.323695 -0.457232 -0.674128
 N7 -1.877972 0.782977 0.089156
 N8 1.695028 0.764107 -0.767720
 N9 1.349729 -1.418063 -0.753691
 N10 -1.018037 -1.426200 -0.275191
 C11 0.150352 -0.837431 -0.439242
 N12 -3.233968 -1.106315 0.211665
 H13 -3.335323 -2.113875 0.164358
 H14 -4.051469 -0.554636 0.437819
 O15 -0.621261 2.710122 -0.127343
 H16 3.354503 -0.622801 -0.952619
 H17 2.186995 1.650511 -0.680246
 O18 1.155060 -0.209964 1.578032
 O19 2.398911 -0.203852 1.256896

Zero-point correction= 0.135528 (Hartree/Particle)
 Thermal correction to Energy= 0.145799
 Thermal correction to Enthalpy= 0.146743
 Thermal correction to Gibbs Free Energy= 0.099956
 Sum of electronic and zero-point Energies= -693.081388
 Sum of electronic and thermal Energies= -693.071117
 Sum of electronic and thermal Enthalpies= -693.070172
 Sum of electronic and thermal Free Energies= -693.116960

5,8-OO-[G + H]⁺

C1 -0.602750 1.456512 -0.136271
 C2 0.545084 0.470335 -0.086978
 H3 -2.644342 1.454527 0.044836
 C4 -2.058424 -0.545737 0.031897
 H5 1.416916 -2.615130 -0.405455
 C6 2.320022 -0.583170 -0.370132
 N7 -1.851044 0.816960 0.010308
 N8 1.652322 0.553246 -0.995317
 N9 1.269841 -1.613075 -0.487163
 N10 -1.085248 -1.464227 -0.120144
 C11 0.122375 -0.978869 -0.263465
 N12 -3.296756 -0.991473 0.197556
 H13 -3.445978 -1.995477 0.201637
 H14 -4.099567 -0.389361 0.335708
 O15 -0.492702 2.645410 -0.263596
 H16 3.302117 -0.868290 -0.739820
 H17 2.181344 1.420936 -0.881775
 O18 1.134566 0.461365 1.261566
 O19 2.421620 -0.235730 1.021765

Zero-point correction= 0.138412 (Hartree/Particle)
 Thermal correction to Energy= 0.147937
 Thermal correction to Enthalpy= 0.148881
 Thermal correction to Gibbs Free Energy= 0.103699
 Sum of electronic and zero-point Energies= -693.109727
 Sum of electronic and thermal Energies= -693.100201

Sum of electronic and thermal Enthalpies= -693.099257
 Sum of electronic and thermal Free Energies= -693.144439

TS1b⁺

C1 -0.799858 1.441829 -0.141974
 C2 0.416771 0.544855 0.164823
 H3 -2.844440 1.272633 -0.108310
 C4 -2.080193 -0.666790 0.020480
 H5 1.502872 -2.448163 -0.560373
 C6 2.395789 -0.427423 -0.412445
 N7 -1.996865 0.711229 -0.043097
 N8 1.662086 0.800590 -0.618395
 N9 1.307675 -1.451361 -0.512981
 N10 -1.031915 -1.496003 -0.126990
 C11 0.142405 -0.914869 -0.210099
 N12 -3.276889 -1.212561 0.188004
 H13 -3.341964 -2.225551 0.206997
 H14 -4.125333 -0.677407 0.330500
 O15 -0.761395 2.617000 -0.375344
 H16 3.059946 -0.470266 -1.331383
 H17 2.190338 1.627254 -0.325252
 O18 0.866722 0.629827 1.412169
 O19 3.202231 -0.547747 0.595341

Zero-point correction= 0.132644 (Hartree/Particle)
 Thermal correction to Energy= 0.142593
 Thermal correction to Enthalpy= 0.143537
 Thermal correction to Gibbs Free Energy= 0.097474
 Sum of electronic and zero-point Energies= -693.046599
 Sum of electronic and thermal Energies= -693.036650
 Sum of electronic and thermal Enthalpies= -693.035706
 Sum of electronic and thermal Free Energies= -693.081768

TS1c⁺

C1 -0.844000 1.393844 -0.271060
 C2 0.304330 0.583396 0.329354
 H3 -2.892837 1.169442 -0.427415
 C4 -2.087091 -0.716965 -0.029866
 H5 1.561459 -2.380970 -0.443418
 C6 2.453081 -0.397630 -0.365191
 N7 -2.042114 0.646079 -0.226226
 N8 1.691898 0.846466 0.032350
 N9 1.359391 -1.397118 -0.277760
 N10 -0.994280 -1.508991 -0.044969
 C11 0.161297 -0.893098 -0.028201
 N12 -3.267295 -1.303760 0.103076
 H13 -3.293740 -2.314023 0.202183
 H14 -4.144057 -0.797132 0.145162
 O15 -0.791799 2.535578 -0.641413
 H16 2.350067 0.183531 -1.417149
 H17 2.120980 1.773985 0.103800
 O18 0.564267 0.846407 1.625426
 O19 3.619935 -0.685841 -0.118848

Zero-point correction= 0.130661 (Hartree/Particle)
 Thermal correction to Energy= 0.141122
 Thermal correction to Enthalpy= 0.142066
 Thermal correction to Gibbs Free Energy= 0.094811
 Sum of electronic and zero-point Energies= -693.060351

Sum of electronic and thermal Energies= -693.049890
 Sum of electronic and thermal Enthalpies= -693.048946
 Sum of electronic and thermal Free Energies= -693.096201

TS1d⁺

C1 -0.755876 1.383525 -0.316727
 C2 0.317403 0.570793 0.397797
 H3 -2.812979 1.209561 -0.546864
 C4 -2.069851 -0.680989 -0.091017
 H5 1.576639 -2.422316 -0.319680
 C6 2.412822 -0.477904 -0.236074
 N7 -1.983086 0.663437 -0.320269
 N8 1.786070 0.815239 0.097502
 N9 1.384315 -1.435439 -0.155329
 N10 -0.981000 -1.502825 -0.057741
 C11 0.161215 -0.895648 0.028868
 N12 -3.255170 -1.255590 0.020957
 H13 -3.293442 -2.263614 0.138935
 H14 -4.127782 -0.739524 0.035826
 O15 -0.666130 2.509844 -0.725252
 H16 2.083593 1.605165 -0.488169
 H17 1.695990 1.019920 1.294754
 O18 0.334021 0.792685 1.732350
 O19 3.560334 -0.652730 -0.495563

Zero-point correction= 0.132807 (Hartree/Particle)
 Thermal correction to Energy= 0.142954
 Thermal correction to Enthalpy= 0.143898
 Thermal correction to Gibbs Free Energy= 0.097172
 Sum of electronic and zero-point Energies= -693.171496
 Sum of electronic and thermal Energies= -693.161349
 Sum of electronic and thermal Enthalpies= -693.160405
 Sum of electronic and thermal Free Energies= -693.207131

5-OH-8-oxoG⁺

C1 -0.718411 1.370720 -0.329665
 C2 0.394277 0.570612 0.358456
 H3 -2.743716 1.179443 -0.677255
 C4 -2.027042 -0.698868 -0.118652
 H5 1.614608 -2.418838 -0.309379
 C6 2.424559 -0.408950 -0.228713
 N7 -1.927793 0.645359 -0.383900
 N8 1.728480 0.779482 -0.102495
 N9 1.409786 -1.443831 -0.104732
 N10 -0.954939 -1.510088 0.000195
 C11 0.205551 -0.918503 0.070169
 N12 -3.227253 -1.256120 -0.054782
 H13 -3.284494 -2.259707 0.088498
 H14 -4.092656 -0.732968 -0.119557
 O15 -0.635772 2.520163 -0.676603
 H16 2.217528 1.667108 -0.067589
 H17 0.333982 1.635950 2.027234
 O18 0.188478 0.710140 1.756359
 O19 3.582691 -0.613385 -0.446197

Zero-point correction= 0.137325 (Hartree/Particle)
 Thermal correction to Energy= 0.148070
 Thermal correction to Enthalpy= 0.149014
 Thermal correction to Gibbs Free Energy= 0.101252

Sum of electronic and zero-point Energies= -693.247473
 Sum of electronic and thermal Energies= -693.236728
 Sum of electronic and thermal Enthalpies= -693.235784
 Sum of electronic and thermal Free Energies= -693.283546

TS1e⁺_1

C1 -0.761933 1.351210 -0.388169
 C2 0.430121 0.549031 0.126340
 H3 -2.784950 1.126882 -0.659102
 C4 -2.059649 -0.729995 -0.036322
 H5 1.560226 -2.495574 -0.129764
 C6 2.391092 -0.445948 -0.292962
 N7 -1.958911 0.603653 -0.372994
 N8 1.744132 0.782201 -0.251357
 N9 1.364025 -1.501378 -0.038675
 N10 -0.999310 -1.531336 0.151778
 C11 0.178701 -0.952127 0.113572
 N12 -3.267610 -1.270674 0.055348
 H13 -3.334045 -2.263503 0.257894
 H14 -4.128557 -0.752727 -0.075713
 O15 -0.737637 2.511703 -0.700825
 H16 1.670331 1.334361 1.088141
 H17 0.141496 1.881149 1.910948
 O18 0.655034 1.083925 1.644712
 O19 3.536256 -0.725736 -0.485870

Zero-point correction= 0.130721 (Hartree/Particle)
 Thermal correction to Energy= 0.141294
 Thermal correction to Enthalpy= 0.142238
 Thermal correction to Gibbs Free Energy= 0.094626
 Sum of electronic and zero-point Energies= -693.153221
 Sum of electronic and thermal Energies= -693.142648
 Sum of electronic and thermal Enthalpies= -693.141704
 Sum of electronic and thermal Free Energies= -693.189317

TS1e⁺_2

C1 0.601063 0.407872 0.916590
 C2 0.087812 -0.733115 0.214543
 C3 -2.123733 -0.524924 -0.071761
 C4 -0.533031 1.090209 -0.761192
 C5 2.342813 -0.565577 -0.212975
 N6 -1.844003 0.716260 -0.665339
 N7 -1.139179 -1.286128 0.319201
 O8 -0.006225 1.974990 -1.354950
 N9 1.168375 -1.313481 -0.401659
 N10 -3.402901 -0.900502 0.014961
 H11 -4.175790 -0.282495 -0.191123
 H12 -3.612528 -1.799882 0.432615
 O13 3.432877 -0.742757 -0.676818
 N14 1.931878 0.488734 0.653491
 H15 1.115457 -2.082999 -1.060743
 O16 -0.050825 1.007034 1.906686
 H17 2.559641 1.257298 0.867584
 H18 -2.536841 1.201919 -1.233759
 H19 0.394700 1.811045 2.230259

Zero-point correction= 0.134183 (Hartree/Particle)
 Thermal correction to Energy= 0.145303
 Thermal correction to Enthalpy= 0.146248

Thermal correction to Gibbs Free Energy= 0.097803
 Sum of electronic and zero-point Energies= -693.197397
 Sum of electronic and thermal Energies= -693.186277
 Sum of electronic and thermal Enthalpies= -693.185333
 Sum of electronic and thermal Free Energies= -693.233778

[Sp + H]⁺

C1 -0.868511 1.031765 -0.467591
 C2 -0.003619 -0.160296 -0.075532
 C3 2.150951 -0.397089 -0.448536
 C4 0.778978 0.168305 1.269960
 C5 -2.306292 -0.737334 -0.110989
 N6 2.092231 -0.027507 0.902669
 N7 0.994485 -0.482848 -1.052437
 O8 0.314688 0.498121 2.328909
 N9 -1.040756 -1.162107 0.120223
 N10 3.329590 -0.634951 -1.032747
 H11 4.210449 -0.584279 -0.540990
 H12 3.339459 -0.914814 -2.005884
 O13 -3.376737 -1.265772 -0.082269
 N14 -2.129127 0.706000 -0.461428
 H15 -0.835466 -2.144028 0.263440
 O16 -0.307761 2.165995 -0.740105
 H17 -2.939513 1.283970 -0.679698
 H18 2.867779 0.057965 1.550808
 H19 -0.918235 2.892218 -0.977782

Zero-point correction= 0.135926 (Hartree/Particle)
 Thermal correction to Energy= 0.147298
 Thermal correction to Enthalpy= 0.148242
 Thermal correction to Gibbs Free Energy= 0.098603
 Sum of electronic and zero-point Energies= -693.230980
 Sum of electronic and thermal Energies= -693.219608
 Sum of electronic and thermal Enthalpies= -693.218663
 Sum of electronic and thermal Free Energies= -693.268303

TS2a⁺

C1 -0.949218 1.483650 -0.093390
 C2 0.121427 0.530074 -0.298860
 C3 -2.329915 -0.561627 0.185009
 C4 2.060804 -0.549920 -0.615464
 N5 -2.168200 0.801981 0.171074
 N6 1.418740 0.711070 -0.614323
 N7 1.015180 -1.489577 -0.604164
 N8 -1.328029 -1.425458 -0.048206
 C9 -0.154458 -0.865764 -0.277480
 N10 -3.539021 -1.065443 0.440841
 H11 -3.645486 -2.073664 0.449322
 H12 -4.354349 -0.497708 0.633518
 O13 -0.870832 2.694938 -0.121212
 H14 2.849547 -0.704691 -1.349661
 H15 1.933682 1.585991 -0.552236
 O16 2.895512 -0.658101 0.749922
 O17 3.567712 0.440430 0.908449
 H18 -2.959166 1.419155 0.341904
 H19 1.154106 -2.493712 -0.635568

Zero-point correction= 0.133999 (Hartree/Particle)
 Thermal correction to Energy= 0.144724

Thermal correction to Enthalpy=	0.145668
Thermal correction to Gibbs Free Energy=	0.097388
Sum of electronic and zero-point Energies=	-693.052485
Sum of electronic and thermal Energies=	-693.041760
Sum of electronic and thermal Enthalpies=	-693.040816
Sum of electronic and thermal Free Energies=	-693.089096

8-OO[G + H]⁺

C1	-0.960396	1.474443	-0.126867
C2	0.168016	0.569138	-0.308486
C3	-2.238397	-0.633270	0.116768
C4	2.248720	-0.448984	-0.642452
N5	-2.156569	0.738798	0.066026
N6	1.455173	0.816685	-0.349672
N7	1.161634	-1.442716	-0.449621
N8	-1.187355	-1.457609	-0.048477
C9	-0.025524	-0.869475	-0.251607
N10	-3.425104	-1.192528	0.332800
H11	-3.476132	-2.205147	0.372373
H12	-4.278209	-0.665806	0.475598
O13	-0.928823	2.684307	-0.131252
H14	2.644094	-0.516763	-1.663598
H15	1.876634	1.742773	-0.437636
O16	3.244487	-0.406131	0.264786
O17	2.533566	0.219883	1.354053
H18	-2.985819	1.313436	0.201025
H19	1.336631	-2.442485	-0.429987

Zero-point correction=	0.135994 (Hartree/Particle)
Thermal correction to Energy=	0.146565
Thermal correction to Enthalpy=	0.147509
Thermal correction to Gibbs Free Energy=	0.099825
Sum of electronic and zero-point Energies=	-693.056359
Sum of electronic and thermal Energies=	-693.045789
Sum of electronic and thermal Enthalpies=	-693.044845
Sum of electronic and thermal Free Energies=	-693.092529

TS2b⁺

C1	1.202081	1.472464	-0.011299
C2	0.005713	0.629252	-0.053331
C3	2.381845	-0.711390	0.034275
C4	-2.099922	-0.250754	0.084257
N5	2.363463	0.669638	0.022366
N6	-1.274564	0.939953	-0.057614
N7	-1.114266	-1.298035	-0.079374
N8	1.277468	-1.470058	0.011147
C9	0.135019	-0.807176	-0.042216
N10	3.561801	-1.326952	0.070160
H11	3.572131	-2.341427	0.080425
H12	4.450652	-0.842015	0.072999
O13	1.226548	2.682657	-0.007973
H14	-2.595188	-0.228655	1.152658
H15	-1.675958	1.878841	-0.082875
O16	-3.220452	-0.332870	-0.640367
O17	-4.139051	-0.096871	0.517112
H18	3.233957	1.196707	0.057859
H19	-1.367678	-2.282980	-0.068158

Zero-point correction=	0.131824 (Hartree/Particle)
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Thermal correction to Energy=	0.142275
Thermal correction to Enthalpy=	0.143219
Thermal correction to Gibbs Free Energy=	0.095498
Sum of electronic and zero-point Energies=	-693.031843
Sum of electronic and thermal Energies=	-693.021393
Sum of electronic and thermal Enthalpies=	-693.020449
Sum of electronic and thermal Free Energies=	-693.068169

8-OOHG⁺

C1	1.070682	1.484789	0.007338
C2	-0.006843	0.538997	0.012641
C3	2.459184	-0.595404	-0.008281
C4	-1.956845	-0.490587	0.023323
N5	2.308344	0.773499	-0.002907
N6	-1.395737	0.714011	0.025334
N7	-1.005752	-1.446828	0.008684
N8	1.426495	-1.436848	-0.003210
C9	0.246145	-0.816716	0.006933
N10	3.704694	-1.099463	-0.018398
H11	3.814503	-2.105311	-0.025529
H12	4.537155	-0.527323	-0.029508
O13	1.021944	2.700383	0.011787
H14	-4.814385	0.189145	0.347070
H15	-1.900601	1.595179	0.023215
O16	-3.247150	-0.801989	0.035834
O17	-3.990884	0.434172	-0.125172
H18	3.125396	1.379030	-0.006272
H19	-1.173589	-2.448310	-0.006812

Zero-point correction=	0.136461 (Hartree/Particle)
Thermal correction to Energy=	0.147921
Thermal correction to Enthalpy=	0.148865
Thermal correction to Gibbs Free Energy=	0.099227
Sum of electronic and zero-point Energies=	-693.159535
Sum of electronic and thermal Energies=	-693.148076
Sum of electronic and thermal Enthalpies=	-693.147132
Sum of electronic and thermal Free Energies=	-693.196770

TS2c⁺_1

C1	-1.201159	1.460133	0.036486
C2	-0.005151	0.628998	-0.099300
H3	-3.207731	1.139105	0.255289
C4	-2.329952	-0.758771	0.088968
H5	4.196729	-1.043729	1.106489
C6	2.006301	-0.179539	-0.485527
N7	-2.330422	0.633640	0.151031
N8	1.276694	0.977940	-0.294766
N9	1.159675	-1.310463	-0.313761
N10	-1.235885	-1.484498	-0.075645
C11	-0.098337	-0.781342	-0.153903
N12	-3.513735	-1.376582	0.200315
H13	-3.525206	-2.389038	0.165244
H14	-4.389275	-0.894333	0.350452
O15	-1.239171	2.672675	0.051917
H16	1.658802	-0.872539	-1.500708
H17	1.660181	1.923356	-0.299231
O18	3.636326	-0.240344	1.071800
O19	3.338094	-0.202324	-0.382230

Zero-point correction= 0.130442 (Hartree/Particle)
 Thermal correction to Energy= 0.141397
 Thermal correction to Enthalpy= 0.142341
 Thermal correction to Gibbs Free Energy= 0.093668
 Sum of electronic and zero-point Energies= -693.050442
 Sum of electronic and thermal Energies= -693.039487
 Sum of electronic and thermal Enthalpies= -693.038543
 Sum of electronic and thermal Free Energies= -693.087216

TS2c⁺_2

C1 -1.215297 1.477981 0.033205
 C2 0.000614 0.678528 -0.089382
 H3 -3.228291 1.101205 0.257415
 C4 -2.323040 -0.764092 0.090823
 C5 2.007008 -0.089555 -0.454716
 N6 -2.344621 0.607458 0.151402
 N7 1.285253 1.080104 -0.185175
 N8 1.168141 -1.182059 -0.394977
 N9 -1.199330 -1.477354 -0.086306
 C10 -0.108384 -0.736751 -0.168929
 N11 -3.473396 -1.430361 0.207558
 H12 -3.447868 -2.442446 0.162181
 H13 -4.367465 -0.981563 0.358208
 O14 -1.340497 2.678022 0.048211
 H15 1.785890 0.859999 -1.380580
 O16 3.663866 -0.396644 1.045416
 O17 3.337065 -0.195145 -0.390596
 H18 4.295954 0.341511 1.173777
 H19 1.460570 -2.149747 -0.508770

Zero-point correction= 0.130687 (Hartree/Particle)
 Thermal correction to Energy= 0.141522
 Thermal correction to Enthalpy= 0.142466
 Thermal correction to Gibbs Free Energy= 0.093965
 Sum of electronic and zero-point Energies= -693.065772
 Sum of electronic and thermal Energies= -693.054937
 Sum of electronic and thermal Enthalpies= -693.053993
 Sum of electronic and thermal Free Energies= -693.102494

TS2c⁺_1'

C1 -1.062820 1.484735 0.105329
 C2 0.141804 0.747384 -0.321053
 H3 -3.032075 1.057201 0.481360
 C4 -2.099805 -0.757122 0.005980
 H5 1.736563 -1.605236 0.330845
 C6 2.246936 -0.026052 -0.699764
 N7 -2.158075 0.610894 0.209614
 N8 1.348078 1.170233 -0.564484
 N9 1.356925 -1.164793 -0.711153
 N10 -0.985838 -1.423806 -0.327536
 C11 0.107774 -0.704603 -0.492727
 N12 -3.216810 -1.461044 0.158178
 H13 -3.167276 -2.465267 0.015704
 H14 -4.110376 -1.058713 0.414796
 O15 -1.123746 2.673647 0.317650
 H16 2.926319 0.089019 -1.543777
 H17 1.680798 2.127965 -0.440067
 O18 2.307996 -0.908013 1.399560
 O19 3.009844 -0.107058 0.508067

Zero-point correction= 0.131711 (Hartree/Particle)
 Thermal correction to Energy= 0.141783
 Thermal correction to Enthalpy= 0.142727
 Thermal correction to Gibbs Free Energy= 0.095855
 Sum of electronic and zero-point Energies= -693.047518
 Sum of electronic and thermal Energies= -693.037446
 Sum of electronic and thermal Enthalpies= -693.036502
 Sum of electronic and thermal Free Energies= -693.083374

TS2c⁺_2'

C1 -0.938422 1.474505 -0.147257
 C2 0.175039 0.534450 -0.349412
 H3 -2.960548 1.373750 0.210327
 C4 -2.272890 -0.595225 0.136271
 C5 2.189934 -0.513106 -0.642747
 N6 -2.149440 0.773906 0.072193
 N7 1.449087 0.774422 -0.488969
 N8 1.111295 -1.507155 -0.357031
 N9 -1.244788 -1.452750 -0.001149
 C10 -0.067000 -0.907942 -0.228462
 N11 -3.476341 -1.115155 0.349882
 H12 -3.557813 -2.125325 0.406575
 H13 -4.316554 -0.561889 0.469102
 O14 -0.873820 2.679865 -0.155639
 H15 2.564597 -0.680745 -1.659404
 O16 2.711963 0.345521 1.316201
 O17 3.239226 -0.419248 0.225005
 H18 2.036784 1.386756 0.178259
 H19 1.265924 -2.510606 -0.324245

Zero-point correction= 0.132907 (Hartree/Particle)
 Thermal correction to Energy= 0.143215
 Thermal correction to Enthalpy= 0.144159
 Thermal correction to Gibbs Free Energy= 0.096889
 Sum of electronic and zero-point Energies= -693.049764
 Sum of electronic and thermal Energies= -693.039455
 Sum of electronic and thermal Enthalpies= -693.038511
 Sum of electronic and thermal Free Energies= -693.085781

8-OOHG⁺_1

C1 -1.138076 1.470758 0.038602
 C2 0.085089 0.664540 -0.257206
 H3 -3.110057 1.113278 0.390017
 C4 -2.201920 -0.769182 0.080063
 H5 3.234076 -1.178800 1.671868
 C6 2.131375 -0.224069 -0.751949
 N7 -2.232919 0.636301 0.191860
 N8 1.287622 1.050570 -0.456464
 N9 1.211149 -1.300912 -0.606799
 N10 -1.130155 -1.481448 -0.184375
 C11 0.029790 -0.819065 -0.358376
 N12 -3.372291 -1.389948 0.261984
 H13 -3.384990 -2.401444 0.188952
 H14 -4.239861 -0.916569 0.476907
 O15 -1.153206 2.677793 0.123085
 H16 2.492394 -0.126328 -1.785324
 H17 1.632649 2.012468 -0.420309
 O18 2.838413 -0.321533 1.415960

O19 3.264092 -0.236566 0.026911

Zero-point correction= 0.135034 (Hartree/Particle)
 Thermal correction to Energy= 0.146115
 Thermal correction to Enthalpy= 0.147060
 Thermal correction to Gibbs Free Energy= 0.098149
 Sum of electronic and zero-point Energies= -693.099650
 Sum of electronic and thermal Energies= -693.088568
 Sum of electronic and thermal Enthalpies= -693.087624
 Sum of electronic and thermal Free Energies= -693.136535

8-OOHG⁺_2

C1 -1.084951 1.495111 -0.023760
 C2 0.131601 0.677804 -0.300773
 H3 -3.080414 1.166299 0.355032
 C4 -2.222171 -0.715547 0.114382
 C5 2.137265 -0.128489 -0.743398
 N6 -2.218361 0.658284 0.166762
 N7 1.327747 1.072815 -0.499804
 N8 1.192005 -1.262892 -0.592952
 N9 -1.134329 -1.471430 -0.133645
 C10 -0.019275 -0.802649 -0.331003
 N11 -3.368384 -1.354324 0.319954
 H12 -3.363690 -2.368368 0.281066
 H13 -4.245106 -0.888348 0.520274
 O14 -1.163147 2.692481 0.041046
 H15 2.534136 -0.086628 -1.765816
 O16 2.792416 -0.279738 1.440071
 O17 3.255597 -0.243476 0.056847
 H18 3.368622 0.409550 1.825543
 H19 1.461959 -2.241191 -0.634713

Zero-point correction= 0.136161 (Hartree/Particle)
 Thermal correction to Energy= 0.147060
 Thermal correction to Enthalpy= 0.148004
 Thermal correction to Gibbs Free Energy= 0.099404
 Sum of electronic and zero-point Energies= -693.124696
 Sum of electronic and thermal Energies= -693.113797
 Sum of electronic and thermal Enthalpies= -693.112852
 Sum of electronic and thermal Free Energies= -693.161452

TS2d⁺_1

C1 1.281618 1.451216 0.026769
 C2 0.063252 0.645540 -0.093791
 H3 3.285801 1.091798 0.152715
 C4 2.354076 -0.792171 0.042272
 H5 -4.598969 0.307452 0.772856
 C6 -1.963462 -0.181044 -0.100486
 N7 2.394327 0.608975 0.068384
 N8 -1.207746 1.019117 -0.154078
 N9 -1.143858 -1.272180 -0.184639
 N10 1.247857 -1.499504 -0.028373
 C11 0.101895 -0.790752 -0.095551
 N12 3.539075 -1.421664 0.101550
 H13 3.536209 -2.434081 0.073222
 H14 4.430399 -0.946432 0.120272
 O15 1.332370 2.664377 0.084176
 H16 -2.810806 -0.323172 1.096816
 H17 -1.555156 1.976174 -0.174948

O18 -3.991249 -0.464809 0.648525

O19 -3.231039 -0.163528 -0.649715

Zero-point correction= 0.128868 (Hartree/Particle)
 Thermal correction to Energy= 0.139651
 Thermal correction to Enthalpy= 0.140595
 Thermal correction to Gibbs Free Energy= 0.092439
 Sum of electronic and zero-point Energies= -693.034726
 Sum of electronic and thermal Energies= -693.023944
 Sum of electronic and thermal Enthalpies= -693.023000
 Sum of electronic and thermal Free Energies= -693.071155

TS2d⁺_2

C1 1.228013 1.482552 0.002239
 C2 0.009558 0.656437 -0.068232
 H3 3.258768 1.163169 0.100108
 C4 2.391726 -0.727943 0.053321
 C5 -1.981369 -0.135656 -0.074092
 N6 2.383523 0.646733 0.048920
 N7 -1.241513 1.028382 -0.154735
 N8 -1.096945 -1.263017 -0.129106
 N9 1.284483 -1.481947 0.002388
 C10 0.158380 -0.788692 -0.063076
 N11 3.569033 -1.354836 0.111193
 H12 3.571953 -2.368146 0.109964
 H13 4.458718 -0.874172 0.139550
 O14 1.321919 2.683946 0.023856
 H15 -2.901890 -0.036033 1.083745
 O16 -4.070339 -0.037794 0.622265
 O17 -3.197683 -0.235301 -0.682095
 H18 -4.585438 -0.876348 0.733430
 H19 -1.361187 -2.242657 -0.130591

Zero-point correction= 0.128959 (Hartree/Particle)
 Thermal correction to Energy= 0.139683
 Thermal correction to Enthalpy= 0.140627
 Thermal correction to Gibbs Free Energy= 0.092664
 Sum of electronic and zero-point Energies= -693.052651
 Sum of electronic and thermal Energies= -693.041928
 Sum of electronic and thermal Enthalpies= -693.040984
 Sum of electronic and thermal Free Energies= -693.088947

ring-opened product

C1 1.094380 1.400858 -0.000002
 C2 -0.316842 0.858656 -0.000002
 H3 3.049820 0.750732 0.000010
 C4 1.809315 -0.929174 0.000005
 C5 -2.828099 -0.641662 -0.000008
 N6 2.089939 0.407948 0.000006
 N7 -1.355163 1.585154 0.000002
 N8 -1.702064 -1.173446 -0.000047
 N9 0.558666 -1.442599 -0.000011
 C10 -0.474226 -0.634725 -0.000013
 N11 2.802606 -1.804372 0.000018
 H12 2.564551 -2.792348 0.000013
 H13 3.783684 -1.547822 0.000031
 O14 1.358801 2.576250 -0.000005
 H15 -1.138221 2.590882 -0.000010
 O16 -3.949411 -0.367996 0.000041

Zero-point correction= 0.108217 (Hartree/Particle)
 Thermal correction to Energy= 0.118160
 Thermal correction to Enthalpy= 0.119104
 Thermal correction to Gibbs Free Energy= 0.072259
 Sum of electronic and zero-point Energies= -616.803094
 Sum of electronic and thermal Energies= -616.793150
 Sum of electronic and thermal Enthalpies= -616.792206
 Sum of electronic and thermal Free Energies= -616.839051

8-oxo[G - H]⁺

C1 0.741895 1.493284 -0.000001
 C2 -0.485045 0.646036 0.000000
 H3 2.785473 1.216904 0.000003
 C4 1.946379 -0.683878 0.000000
 C5 -2.479644 -0.231402 0.000001
 N6 1.917254 0.683355 0.000001
 N7 -1.710538 1.008069 0.000002
 N8 -1.543467 -1.327181 -0.000002
 N9 0.837003 -1.473225 -0.000002
 C10 -0.301451 -0.838200 -0.000002
 N11 3.111721 -1.311095 0.000002
 H12 3.109639 -2.327109 0.000003
 H13 4.008131 -0.836691 0.000005
 O14 0.803002 2.691265 -0.000002
 O15 -3.665276 -0.331620 0.000002
 H16 -1.821670 -2.304749 -0.000003

Zero-point correction= 0.109534 (Hartree/Particle)
 Thermal correction to Energy= 0.118602
 Thermal correction to Enthalpy= 0.119547
 Thermal correction to Gibbs Free Energy= 0.075085
 Sum of electronic and zero-point Energies= -616.805993
 Sum of electronic and thermal Energies= -616.796925
 Sum of electronic and thermal Enthalpies= -616.795980
 Sum of electronic and thermal Free Energies= -616.840442

[G + H]⁺(H₂O)

C1 0.106541 -1.211296 0.000334
 C2 0.479414 0.175822 0.000242
 H3 -1.642926 -2.279911 0.000154
 C4 -2.202459 -0.268805 -0.000115
 H5 -0.233580 3.285835 -0.000175
 C6 1.523037 2.111984 0.000193
 N7 -1.305315 -1.320583 0.000133
 N8 1.713683 0.801120 0.000355
 N9 0.193210 2.364881 -0.000006
 N10 -1.824447 1.004393 -0.000170
 C11 -0.496938 1.161227 0.000009
 N12 -3.514029 -0.560682 -0.000290
 H13 -4.174079 0.206404 -0.000514
 H14 -3.876979 -1.503337 -0.000330
 O15 0.823406 -2.203489 0.000548
 H16 2.299214 2.863268 0.000184
 H17 2.613927 0.271149 0.000474
 O18 3.487795 -1.194647 -0.001564
 H19 2.842583 -1.929882 -0.000135
 H20 4.382951 -1.565925 0.004340

Zero-point correction= 0.154172 (Hartree/Particle)
 Thermal correction to Energy= 0.165790
 Thermal correction to Enthalpy= 0.166734
 Thermal correction to Gibbs Free Energy= 0.116671
 Sum of electronic and zero-point Energies= -619.247869
 Sum of electronic and thermal Energies= -619.236252
 Sum of electronic and thermal Enthalpies= -619.235307
 Sum of electronic and thermal Free Energies= -619.285371

PC⁺(H₂O)

C1 -0.245842 1.428980 0.021716
 C2 0.298575 0.153590 -0.376628
 H3 -2.101754 2.182670 0.458877
 C4 -2.402195 0.184869 -0.067304
 H5 -0.015724 -2.931338 -1.141022
 C6 1.559380 -1.536059 -0.972616
 N7 -1.648484 1.320037 0.167120
 N8 1.577457 -0.238497 -0.672752
 N9 0.278318 -1.974133 -0.972772
 N10 -1.875174 -0.974813 -0.457098
 C11 -0.552125 -0.940584 -0.582063
 N12 -3.728474 0.264197 0.104738
 H13 -4.281302 -0.569224 -0.054156
 H14 -4.204905 1.102828 0.406798
 O15 0.343800 2.479350 0.218406
 H16 2.420159 -2.133249 -1.235033
 H17 2.403119 0.404246 -0.567634
 O18 3.136072 1.898997 -0.335829
 H19 2.437569 2.506230 -0.021585
 H20 3.966191 2.151994 0.097143
 O21 1.626909 -1.673700 1.629208
 O22 0.543766 -1.109206 1.829881

Zero-point correction= 0.159408 (Hartree/Particle)
 Thermal correction to Energy= 0.174062
 Thermal correction to Enthalpy= 0.175006
 Thermal correction to Gibbs Free Energy= 0.117993
 Sum of electronic and zero-point Energies= -769.512367
 Sum of electronic and thermal Energies= -769.497713
 Sum of electronic and thermal Enthalpies= -769.496769
 Sum of electronic and thermal Free Energies= -769.553782

TS1a⁺(H₂O)

C1 -0.248864 1.442942 -0.006685
 C2 0.307975 0.136599 -0.322312
 H3 -2.105352 2.225254 0.382075
 C4 -2.403877 0.205812 -0.059409
 H5 -0.042618 -3.004753 -0.799569
 C6 1.552456 -1.621945 -0.604514
 N7 -1.651339 1.348946 0.135443
 N8 1.555431 -0.243898 -0.647928
 N9 0.249394 -2.032428 -0.812505
 N10 -1.883702 -0.982960 -0.381537
 C11 -0.565781 -0.991008 -0.477026
 N12 -3.727309 0.295848 0.083706
 H13 -4.278829 -0.545144 -0.042734
 H14 -4.209274 1.150510 0.329690
 O15 0.347683 2.493830 0.124349
 H16 2.406759 -2.220927 -0.886467

H17 2.385471 0.380820 -0.503490
 O18 3.230514 1.836270 -0.285301
 H19 2.599299 2.522904 -0.002650
 H20 4.072432 2.013683 0.162661
 O21 1.622131 -1.572142 1.261686
 O22 0.490090 -1.039870 1.591755

Zero-point correction= 0.159657 (Hartree/Particle)
 Thermal correction to Energy= 0.172975
 Thermal correction to Enthalpy= 0.173919
 Thermal correction to Gibbs Free Energy= 0.120233
 Sum of electronic and zero-point Energies= -769.506859
 Sum of electronic and thermal Energies= -769.493541
 Sum of electronic and thermal Enthalpies= -769.492597
 Sum of electronic and thermal Free Energies= -769.546283

5,8-OO-[G + H]⁺(H₂O)

C1 -0.262931 1.393441 0.014785
 C2 0.337122 0.005372 -0.006604
 H3 -2.109613 2.271880 0.131746
 C4 -2.450509 0.222671 -0.051240
 H5 -0.198154 -3.118472 -0.553527
 C6 1.495799 -1.685939 -0.325404
 N7 -1.669660 1.356777 0.058177
 N8 1.430614 -0.338365 -0.854885
 N9 0.109530 -2.150347 -0.568394
 N10 -1.968631 -1.014359 -0.254992
 C11 -0.660019 -1.096304 -0.322365
 N12 -3.768330 0.361766 0.036421
 H13 -4.341920 -0.470468 -0.053967
 H14 -4.232790 1.245880 0.203811
 O15 0.354347 2.426844 0.019973
 H16 2.280909 -2.345916 -0.685787
 H17 2.274588 0.230525 -0.669621
 O18 3.420663 1.639416 -0.323873
 H19 4.377189 1.797546 -0.346072
 H20 3.003022 2.489739 -0.111774
 O21 1.629466 -1.528972 1.102163
 O22 0.752441 -0.367846 1.366220

Zero-point correction= 0.161587 (Hartree/Particle)
 Thermal correction to Energy= 0.175016
 Thermal correction to Enthalpy= 0.175961
 Thermal correction to Gibbs Free Energy= 0.121149
 Sum of electronic and zero-point Energies= -769.527778
 Sum of electronic and thermal Energies= -769.514349
 Sum of electronic and thermal Enthalpies= -769.513405
 Sum of electronic and thermal Free Energies= -769.568216

Cartesian coordinates for the structures in Fig. 3, optimized at B3LYP/6-31+G*.

Fig. 3a

[G – H]⁻

C1 -0.261395 1.429999 -0.003305
 C2 0.767369 0.420465 -0.012285
 C3 -1.695027 -0.436296 -0.017010
 C4 2.618496 -0.774026 0.010544
 N5 -1.531994 0.899252 -0.007369
 N6 2.148527 0.509623 -0.000047
 N7 1.657092 -1.681927 0.007586
 N8 -0.789517 -1.425036 -0.007996
 C9 0.479017 -0.942066 -0.006266
 N10 -3.039529 -0.860042 -0.075627
 H11 -3.165646 -1.784486 0.321237
 H12 -3.669114 -0.166340 0.311352
 O13 -0.010018 2.661510 0.012716
 H14 3.679306 -0.995592 0.018455
 H15 2.672783 1.372798 0.001334

Zero-point correction= 0.103457 (Hartree/Particle)
 Thermal correction to Energy= 0.111428
 Thermal correction to Enthalpy= 0.112372
 Thermal correction to Gibbs Free Energy= 0.070616
 Sum of electronic and zero-point Energies= -541.929698
 Sum of electronic and thermal Energies= -541.921727
 Sum of electronic and thermal Enthalpies= -541.920783
 Sum of electronic and thermal Free Energies= -541.962539

PC⁻

C1 -0.641839 1.434791 -0.247924
 C2 0.421412 0.438981 -0.389181
 C3 -2.008225 -0.446727 0.037967
 C4 2.185211 -0.747939 -0.874687
 N5 -1.869741 0.884940 0.031123
 N6 1.698058 0.548995 -0.866185
 N7 1.254954 -1.672427 -0.730226
 N8 -1.107962 -1.436201 -0.198723
 C9 0.116535 -0.959487 -0.422968
 N10 -3.297253 -0.903197 0.283581
 H11 -3.341251 -1.853328 0.629198
 H12 -3.885454 -0.233207 0.761962
 O13 -0.430930 2.653381 -0.374112
 H14 3.220457 -0.953316 -1.113742
 H15 2.272314 1.357132 -0.659159
 O16 2.383974 -0.088309 1.498837
 O17 1.115577 0.111208 1.640964

Zero-point correction= 0.109221 (Hartree/Particle)
 Thermal correction to Energy= 0.120001
 Thermal correction to Enthalpy= 0.120945
 Thermal correction to Gibbs Free Energy= 0.072755
 Sum of electronic and zero-point Energies= -692.221542
 Sum of electronic and thermal Energies= -692.210761
 Sum of electronic and thermal Enthalpies= -692.209817
 Sum of electronic and thermal Free Energies= -692.258007

TS1⁻

C1 -0.635082 1.431746 -0.215450
 C2 0.463845 0.439895 -0.264357
 C3 -2.000894 -0.451545 0.021588
 C4 2.208276 -0.732830 -0.754451
 N5 -1.867038 0.882279 0.023195
 N6 1.705207 0.562237 -0.860553
 N7 1.268237 -1.672532 -0.675251
 N8 -1.096720 -1.441348 -0.206405
 C9 0.134456 -0.972537 -0.390700
 N10 -3.288153 -0.908848 0.239253
 H11 -3.350651 -1.867943 0.554324
 H12 -3.901745 -0.242796 0.689328
 O13 -0.424928 2.643354 -0.366966
 H14 3.245932 -0.943753 -0.978693
 H15 2.287738 1.342928 -0.576444
 O16 2.333813 -0.153432 1.404537
 O17 1.046664 0.193913 1.498683

Zero-point correction= 0.109043 (Hartree/Particle)
 Thermal correction to Energy= 0.118992
 Thermal correction to Enthalpy= 0.119936
 Thermal correction to Gibbs Free Energy= 0.073507
 Sum of electronic and zero-point Energies= -692.220746
 Sum of electronic and thermal Energies= -692.210797
 Sum of electronic and thermal Enthalpies= -692.209853
 Sum of electronic and thermal Free Energies= -692.256282

5,8-OO-[G – H]⁻

C1 -0.649237 1.422308 -0.129160
 C2 0.509509 0.426583 -0.082372
 C3 -2.024538 -0.464442 0.016783
 C4 2.232874 -0.691045 -0.409921
 N5 -1.885461 0.880781 -0.004642
 N6 1.619093 0.507183 -1.008070
 N7 1.228278 -1.728879 -0.474613
 N8 -1.134109 -1.463990 -0.125251
 C9 0.133858 -1.038882 -0.258825
 N10 -3.332458 -0.883957 0.161194
 H11 -3.448460 -1.840001 0.469137
 H12 -3.966025 -0.192937 0.539356
 O13 -0.410399 2.627534 -0.263491
 H14 3.223113 -0.961842 -0.776503
 H15 2.164432 1.348396 -0.807153
 O16 2.416619 -0.287240 1.002488
 O17 1.161873 0.477366 1.250479

Zero-point correction= 0.112125 (Hartree/Particle)
 Thermal correction to Energy= 0.121204
 Thermal correction to Enthalpy= 0.122148
 Thermal correction to Gibbs Free Energy= 0.077788
 Sum of electronic and zero-point Energies= -692.243078
 Sum of electronic and thermal Energies= -692.233999
 Sum of electronic and thermal Enthalpies= -692.233055
 Sum of electronic and thermal Free Energies= -692.277415

TS2a⁻

C1 -1.016523 1.452551 -0.059929
 C2 0.036679 0.466879 -0.335457

C3 -2.364031 -0.454313 0.158099
 C4 1.908594 -0.701416 -0.598702
 N5 -2.239064 0.889398 0.167093
 N6 1.335163 0.599807 -0.581503
 N7 0.922550 -1.636771 -0.476511
 N8 -1.451108 -1.429025 -0.029000
 C9 -0.219093 -0.951502 -0.278113
 N10 -3.658643 -0.907466 0.353511
 H11 -3.730365 -1.866619 0.666984
 H12 -4.276272 -0.240412 0.796803
 O13 -0.776404 2.674595 -0.064935
 H14 2.755916 -0.878673 -1.248504
 H15 1.871376 1.454920 -0.474003
 O16 2.930005 -0.473352 0.864309
 O17 3.964311 0.304506 0.564151

Zero-point correction= 0.108313 (Hartree/Particle)
 Thermal correction to Energy= 0.118556
 Thermal correction to Enthalpy= 0.119500
 Thermal correction to Gibbs Free Energy= 0.071797
 Sum of electronic and zero-point Energies= -692.203445
 Sum of electronic and thermal Energies= -692.193201
 Sum of electronic and thermal Enthalpies= -692.192257
 Sum of electronic and thermal Free Energies= -692.239960

8-OO[G - H]⁻

C1 1.092855 1.461722 -0.004491
 C2 -0.047340 0.513855 0.166995
 C3 2.370184 -0.504633 -0.051766
 C4 -2.018952 -0.626927 0.341880
 N5 2.299325 0.853452 -0.087636
 N6 -1.318627 0.711141 0.263178
 N7 -0.975017 -1.595925 0.156160
 N8 1.419230 -1.446229 0.040699
 C9 0.166522 -0.951057 0.142243
 N10 3.658781 -0.985784 -0.099299
 H11 3.760131 -1.961731 -0.342007
 H12 4.358944 -0.339634 -0.435809
 O13 0.882323 2.684322 -0.034432
 H14 -2.464792 -0.688700 1.351386
 H15 -1.851941 1.573707 0.179359
 O16 -3.010049 -0.632856 -0.612571
 O17 -3.968249 0.361287 -0.132224

Zero-point correction= 0.109064 (Hartree/Particle)
 Thermal correction to Energy= 0.119378
 Thermal correction to Enthalpy= 0.120322
 Thermal correction to Gibbs Free Energy= 0.072847
 Sum of electronic and zero-point Energies= -692.217001
 Sum of electronic and thermal Energies= -692.206687
 Sum of electronic and thermal Enthalpies= -692.205743
 Sum of electronic and thermal Free Energies= -692.253218

TS2b⁻

C1 1.233453 1.434713 -0.002978
 C2 0.032538 0.582280 -0.098609
 C3 2.353165 -0.629196 0.059216
 C4 -2.008212 -0.352060 -0.012870
 N5 2.392112 0.729184 0.053974

N6 -1.247776 0.886269 -0.167386
 N7 -1.092966 -1.406203 -0.100757
 N8 1.322211 -1.482045 0.015247
 C9 0.121609 -0.858814 -0.062334
 N10 3.602730 -1.219603 0.164154
 H11 3.643383 -2.186258 -0.130978
 H12 4.374307 -0.629001 -0.115529
 O13 1.129947 2.676456 0.003166
 H14 -2.574264 -0.241523 1.081456
 H15 -1.640355 1.821172 -0.128694
 O16 -3.228939 -0.406511 -0.611581
 O17 -4.030080 -0.067338 0.638736

Zero-point correction= 0.105427 (Hartree/Particle)
 Thermal correction to Energy= 0.115372
 Thermal correction to Enthalpy= 0.116317
 Thermal correction to Gibbs Free Energy= 0.069567
 Sum of electronic and zero-point Energies= -692.201175
 Sum of electronic and thermal Energies= -692.191230
 Sum of electronic and thermal Enthalpies= -692.190286
 Sum of electronic and thermal Free Energies= -692.237036

8-OOH[G - 2H]⁻

C1 1.303530 1.416567 0.056158
 C2 0.082759 0.624122 -0.088295
 C3 2.336010 -0.689509 0.105139
 C4 -1.943316 -0.206446 -0.425004
 N5 2.433018 0.656680 0.159482
 N6 -1.201228 0.975711 -0.241000
 N7 -1.136055 -1.293935 -0.347071
 N8 1.268584 -1.491826 -0.057649
 C9 0.111233 -0.806013 -0.157084
 N10 3.544655 -1.354900 0.272062
 H11 3.555312 -2.300723 -0.087464
 H12 4.359900 -0.792188 0.066679
 O13 1.269228 2.664581 0.072065
 H14 -4.058947 -1.230974 0.996977
 H15 -1.578875 1.914924 -0.223440
 O16 -3.195440 -0.165924 -0.620729
 O17 -4.071475 -0.256842 1.023788

Zero-point correction= 0.107868 (Hartree/Particle)
 Thermal correction to Energy= 0.119091
 Thermal correction to Enthalpy= 0.120036
 Thermal correction to Gibbs Free Energy= 0.070479
 Sum of electronic and zero-point Energies= -692.286171
 Sum of electronic and thermal Energies= -692.274947
 Sum of electronic and thermal Enthalpies= -692.274003
 Sum of electronic and thermal Free Energies= -692.323560

TS2c⁻

C1 -1.218628 1.438443 0.009030
 C2 -0.001290 0.616001 -0.095827
 C3 -2.313717 -0.644623 0.092711
 C4 1.933826 -0.287304 -0.470160
 N5 -2.370240 0.694062 0.144054
 N6 1.291836 0.990264 -0.219222
 N7 1.127093 -1.358151 -0.378900
 N8 -1.266545 -1.479572 -0.073689

C9 -0.102665 -0.812710 -0.170555
 N10 -3.548838 -1.283357 0.188923
 H11 -3.491871 -2.244974 0.499751
 H12 -4.262450 -0.722087 0.635718
 O13 -1.206037 2.679863 -0.008536
 H14 1.739191 0.636461 -1.404527
 O15 3.673207 -0.246610 1.055441
 O16 3.294820 -0.330073 -0.391704
 H17 3.500903 0.703592 1.208087

Zero-point correction= 0.104704 (Hartree/Particle)
 Thermal correction to Energy= 0.114889
 Thermal correction to Enthalpy= 0.115833
 Thermal correction to Gibbs Free Energy= 0.068532
 Sum of electronic and zero-point Energies= -692.203199
 Sum of electronic and thermal Energies= -692.193014
 Sum of electronic and thermal Enthalpies= -692.192070
 Sum of electronic and thermal Free Energies= -692.239371

TS2c₋₁

C1 1.014354 1.469927 0.031127
 C2 -0.105357 0.480053 0.176217
 C3 2.352685 -0.456391 -0.081725
 C4 -1.999587 -0.724930 0.395984
 N5 2.235970 0.897767 -0.088819
 N6 -1.368861 0.630814 0.338144
 N7 -0.938014 -1.679449 0.233785
 N8 1.438464 -1.434205 0.018569
 C9 0.171395 -0.988247 0.145004
 N10 3.653711 -0.891968 -0.172084
 H11 3.784747 -1.861127 -0.426823
 H12 4.326602 -0.215930 -0.504997
 O13 0.776240 2.684270 0.035759
 H14 -2.434596 -0.811106 1.408923
 H15 -2.148802 1.309012 0.109158
 O16 -2.988896 -0.722314 -0.572229
 O17 -3.697067 0.567539 -0.325163

Zero-point correction= 0.107194 (Hartree/Particle)
 Thermal correction to Energy= 0.116932
 Thermal correction to Enthalpy= 0.117876
 Thermal correction to Gibbs Free Energy= 0.071629
 Sum of electronic and zero-point Energies= -692.217816
 Sum of electronic and thermal Energies= -692.208078
 Sum of electronic and thermal Enthalpies= -692.207133
 Sum of electronic and thermal Free Energies= -692.253380

8-OOH[G - 2H]₋₁

C1 1.095529 1.470203 0.024475
 C2 -0.075658 0.533600 0.186945
 C3 2.365193 -0.501733 -0.084684
 C4 -1.941745 -0.557773 0.447203
 N5 2.302628 0.846755 -0.102276
 N6 -1.325917 0.791574 0.313750
 N7 -0.962877 -1.593015 0.282564
 N8 1.413204 -1.449855 0.029055
 C9 0.172356 -0.946401 0.165633
 N10 3.648992 -1.000563 -0.179261
 H11 3.720932 -1.970465 -0.455416

H12 4.337235 -0.357610 -0.545972
 O13 0.943466 2.696498 0.013408
 H14 -2.427515 -0.602577 1.434198
 H15 -3.374021 1.137025 -0.376012
 O16 -2.941680 -0.702124 -0.564737
 O17 -3.937147 0.335871 -0.311303

Zero-point correction= 0.110301 (Hartree/Particle)
 Thermal correction to Energy= 0.120551
 Thermal correction to Enthalpy= 0.121496
 Thermal correction to Gibbs Free Energy= 0.074072
 Sum of electronic and zero-point Energies= -692.259136
 Sum of electronic and thermal Energies= -692.248885
 Sum of electronic and thermal Enthalpies= -692.247941
 Sum of electronic and thermal Free Energies= -692.295365

TS2d⁺

C1 1.304003 1.441060 0.021118
 C2 0.028789 0.646335 -0.096044
 C3 2.351268 -0.658970 0.089791
 C4 -1.949778 -0.215885 -0.232094
 N5 2.440271 0.680823 0.093790
 N6 -1.185120 1.057787 -0.221743
 N7 -1.091945 -1.366707 -0.227562
 N8 1.284483 -1.489856 0.011622
 C9 0.110413 -0.842208 -0.081320
 N10 3.559700 -1.313549 0.210455
 H11 3.566953 -2.281776 -0.079955
 H12 4.378865 -0.756773 0.008639
 O13 1.301786 2.674187 0.050240
 H14 -2.442172 -0.259330 0.874070
 H15 -4.313495 0.664258 0.888142
 O16 -3.123267 -0.207425 -0.816304
 O17 -4.092273 -0.287744 0.895372

Zero-point correction= 0.101475 (Hartree/Particle)
 Thermal correction to Energy= 0.112083
 Thermal correction to Enthalpy= 0.113027
 Thermal correction to Gibbs Free Energy= 0.065057
 Sum of electronic and zero-point Energies= -692.190658
 Sum of electronic and thermal Energies= -692.180050
 Sum of electronic and thermal Enthalpies= -692.179106
 Sum of electronic and thermal Free Energies= -692.227076

8-oxo[G - 3H]⁻

C1 -0.803799 1.451584 -0.001588
 C2 0.459363 0.627099 -0.004197
 C3 -1.901159 -0.615003 -0.007496
 C4 2.414617 -0.334387 0.002203
 N5 -1.965559 0.721369 -0.001899
 N6 1.687137 0.986091 -0.001007
 N7 1.546547 -1.421734 0.000365
 N8 -0.843770 -1.483438 -0.006971
 C9 0.339287 -0.879748 -0.004549
 N10 -3.114363 -1.250559 -0.039681
 H11 -3.122989 -2.237537 0.174276
 H12 -3.930226 -0.692502 0.167127
 O13 -0.776935 2.682674 0.005068
 O14 3.631113 -0.361341 0.007021

Zero-point correction= 0.083262 (Hartree/Particle)
 Thermal correction to Energy= 0.092078
 Thermal correction to Enthalpy= 0.093022
 Thermal correction to Gibbs Free Energy= 0.048904
 Sum of electronic and zero-point Energies= -615.965062
 Sum of electronic and thermal Energies= -615.956246
 Sum of electronic and thermal Enthalpies= -615.955302
 Sum of electronic and thermal Free Energies= -615.999420

Fig. 3b

[G – H]⁻(H₂O)

C1 -0.108650 -1.153082 0.031887
 C2 -0.437003 0.243586 0.010238
 C3 2.103456 -0.384519 -0.029620
 C4 -1.322356 2.251393 0.022327
 N5 1.230686 -1.411599 0.005069
 N6 -1.642340 0.927905 0.033913
 N7 -0.018779 2.487547 -0.002679
 N8 1.881244 0.933937 -0.030087
 C9 0.556653 1.225431 -0.010763
 N10 3.455570 -0.771135 -0.108369
 H11 4.079443 -0.062229 0.260155
 H12 3.611634 -1.691368 0.286458
 O13 -0.980040 -2.082752 0.077339
 H14 -2.084891 3.021393 0.032930
 H15 -2.558640 0.474686 0.032709
 O16 -3.490817 -1.262875 0.011747
 H17 -3.827080 -1.591712 -0.834313
 H18 -2.550883 -1.649188 0.080026

Zero-point correction= 0.128879 (Hartree/Particle)
 Thermal correction to Energy= 0.139193
 Thermal correction to Enthalpy= 0.140137
 Thermal correction to Gibbs Free Energy= 0.092955
 Sum of electronic and zero-point Energies= -618.357689
 Sum of electronic and thermal Energies= -618.347375
 Sum of electronic and thermal Enthalpies= -618.346430
 Sum of electronic and thermal Free Energies= -618.393613

PC⁻(H₂O)

C1 -0.217832 1.369439 0.020870
 C2 0.288837 0.046072 -0.310883
 C3 -2.308033 0.326786 -0.069987
 C4 1.362213 -1.744519 -0.935763
 N5 -1.569512 1.429526 0.160815
 N6 1.522108 -0.403304 -0.675648
 N7 0.100693 -2.143711 -0.958619
 N8 -1.938118 -0.914593 -0.443420
 C9 -0.609305 -1.035333 -0.562468
 N10 -3.679750 0.511915 0.058518
 H11 -4.195630 -0.341311 0.232376
 H12 -3.933561 1.301482 0.638183
 O13 0.531858 2.373318 0.160987
 H14 2.207377 -2.370340 -1.190447
 H15 2.389539 0.109343 -0.502038
 O16 3.158015 1.935692 -0.241342
 H17 3.347545 2.441860 -1.044397

H18 2.211338 2.178633 -0.009920
 O19 1.540572 -1.667935 1.591634
 O20 0.498326 -0.947721 1.742985

Zero-point correction= 0.134329 (Hartree/Particle)
 Thermal correction to Energy= 0.147762
 Thermal correction to Enthalpy= 0.148706
 Thermal correction to Gibbs Free Energy= 0.094467
 Sum of electronic and zero-point Energies= -768.643375
 Sum of electronic and thermal Energies= -768.629942
 Sum of electronic and thermal Enthalpies= -768.628997
 Sum of electronic and thermal Free Energies= -768.683237

TS1⁻(H₂O)

C1 -0.216598 1.366865 0.014875
 C2 0.301603 -0.003675 -0.187202
 C3 -2.312870 0.339971 -0.064401
 C4 1.339626 -1.811768 -0.681356
 N5 -1.561975 1.450050 0.128563
 N6 1.495010 -0.423949 -0.714970
 N7 0.049050 -2.195954 -0.797693
 N8 -1.965018 -0.919859 -0.384324
 C9 -0.637730 -1.083343 -0.478439
 N10 -3.673514 0.555553 0.045842
 H11 -4.224473 -0.275080 0.217175
 H12 -3.931238 1.386944 0.560389
 O13 0.547074 2.359034 0.082064
 H14 2.168142 -2.463705 -0.926276
 H15 2.361125 0.037977 -0.429791
 O16 3.221788 1.928304 -0.213815
 H17 3.395179 2.347091 -1.069239
 H18 2.272749 2.162909 -0.014637
 O19 1.505643 -1.687645 1.335756
 O20 0.564178 -0.762860 1.558445

Zero-point correction= 0.134232 (Hartree/Particle)
 Thermal correction to Energy= 0.146842
 Thermal correction to Enthalpy= 0.147786
 Thermal correction to Gibbs Free Energy= 0.095344
 Sum of electronic and zero-point Energies= -768.639639
 Sum of electronic and thermal Energies= -768.627029
 Sum of electronic and thermal Enthalpies= -768.626085
 Sum of electronic and thermal Free Energies= -768.678526

5,8-OO-[G – H]⁻(H₂O)

C1 -0.206055 1.333444 0.111003
 C2 0.320420 -0.096812 0.037536
 C3 -2.328767 0.376118 -0.074428
 C4 1.301081 -1.874575 -0.397267
 N5 -1.542168 1.472309 0.103840
 N6 1.413904 -0.475278 -0.829733
 N7 -0.074366 -2.262607 -0.642851
 N8 -2.029155 -0.903951 -0.328720
 C9 -0.704567 -1.151251 -0.362671
 N10 -3.675915 0.661164 -0.032968
 H11 -4.287979 -0.130341 0.110771
 H12 -3.924595 1.535855 0.407901
 O13 0.595128 2.286972 0.183710
 H14 2.063474 -2.559780 -0.766695

H15 2.286934 -0.037928 -0.517336
 O16 3.290176 2.004370 -0.345861
 H17 3.258685 2.245616 -1.283164
 H18 2.359287 2.150196 -0.036773
 O19 1.506560 -1.782081 1.065537
 O20 0.771313 -0.530089 1.385776

Zero-point correction= 0.136911 (Hartree/Particle)
 Thermal correction to Energy= 0.149029
 Thermal correction to Enthalpy= 0.149973
 Thermal correction to Gibbs Free Energy= 0.098323
 Sum of electronic and zero-point Energies= -768.660731
 Sum of electronic and thermal Energies= -768.648613
 Sum of electronic and thermal Enthalpies= -768.647669
 Sum of electronic and thermal Free Energies= -768.699319

TS2a⁺(H₂O)

C1 -0.953091 1.324875 0.007581
 C2 -0.092524 0.187510 -0.328949
 C3 -2.626654 -0.305629 0.142585
 C4 1.536967 -1.290882 -0.614983
 N5 -2.251569 0.995603 0.207466
 N6 1.208988 0.091444 -0.581436
 N7 0.389188 -2.039352 -0.515202
 N8 -1.906818 -1.417818 -0.070589
 C9 -0.603233 -1.164861 -0.303268
 N10 -3.985469 -0.507341 0.309595
 H11 -4.248540 -1.447428 0.574603
 H12 -4.474016 0.247836 0.771792
 O13 -0.510012 2.501008 0.090628
 H14 2.334094 -1.604274 -1.278821
 H15 1.870859 0.881725 -0.532253
 O16 2.489634 -1.342291 0.857293
 O17 3.714195 -0.866097 0.655759
 O18 2.178923 2.713516 -0.226281
 H19 2.590124 2.714341 0.651003
 H20 1.196526 2.794892 -0.072136

Zero-point correction= 0.133838 (Hartree/Particle)
 Thermal correction to Energy= 0.146484
 Thermal correction to Enthalpy= 0.147428
 Thermal correction to Gibbs Free Energy= 0.094409
 Sum of electronic and zero-point Energies= -768.624578
 Sum of electronic and thermal Energies= -768.611932
 Sum of electronic and thermal Enthalpies= -768.610988
 Sum of electronic and thermal Free Energies= -768.664007

8-OO[G - H]⁺(H₂O)

C1 -1.115010 1.454556 -0.191445
 C2 -0.142577 0.325371 -0.384007
 C3 -2.644374 -0.282686 0.196386
 C4 1.589657 -1.108232 -0.722125
 N5 -2.373660 1.048289 0.084233
 N6 1.103823 0.334135 -0.683405
 N7 0.438451 -1.899830 -0.321832
 N8 -1.864504 -1.365900 0.087826
 C9 -0.571861 -1.086155 -0.195269
 N10 -3.971541 -0.545725 0.443676
 H11 -4.183833 -1.470543 0.792092

H12 -4.518068 0.229210 0.792550
 O13 -0.727738 2.626089 -0.299351
 H14 1.792252 -1.336568 -1.783204
 H15 1.793069 1.128166 -0.581253
 O16 2.780631 -1.245756 -0.076340
 O17 2.677974 -0.615515 1.261401
 O18 3.162543 1.677770 0.306070
 H19 3.079104 0.739425 0.818749
 H20 2.867193 2.355709 0.932101

Zero-point correction= 0.133134 (Hartree/Particle)
 Thermal correction to Energy= 0.145508
 Thermal correction to Enthalpy= 0.146452
 Thermal correction to Gibbs Free Energy= 0.094319
 Sum of electronic and zero-point Energies= -768.641727
 Sum of electronic and thermal Energies= -768.629353
 Sum of electronic and thermal Enthalpies= -768.628408
 Sum of electronic and thermal Free Energies= -768.680542

TS2b⁺(H₂O)

C1 1.183587 1.256120 0.053423
 C2 0.102536 0.255757 -0.046199
 C3 2.586409 -0.624210 0.037687
 C4 -1.771599 -0.974812 -0.004690
 N5 2.422838 0.729787 0.074478
 N6 -1.210431 0.370456 -0.095190
 N7 -0.703933 -1.880042 -0.137534
 N8 1.690140 -1.607218 -0.028590
 C9 0.409010 -1.159670 -0.072899
 N10 3.910489 -1.019301 0.116936
 H11 4.096516 -1.962743 -0.196470
 H12 4.584260 -0.312362 -0.144286
 O13 0.942077 2.491691 0.089544
 H14 -2.299032 -1.030042 1.089377
 H15 -1.731972 1.258634 -0.048469
 O16 -2.962640 -1.193261 -0.618704
 O17 -3.814278 -1.132167 0.641693
 O18 -1.660963 3.170269 -0.012542
 H19 -0.668207 3.067396 0.040570
 H20 -1.838510 3.611978 -0.855273

Zero-point correction= 0.130889 (Hartree/Particle)
 Thermal correction to Energy= 0.143357
 Thermal correction to Enthalpy= 0.144301
 Thermal correction to Gibbs Free Energy= 0.091889
 Sum of electronic and zero-point Energies= -768.621064
 Sum of electronic and thermal Energies= -768.608596
 Sum of electronic and thermal Enthalpies= -768.607652
 Sum of electronic and thermal Free Energies= -768.660064

8-OOH[G - 2H]⁺(H₂O)

C1 1.286378 1.182237 0.031556
 C2 0.139875 0.316911 -0.070495
 C3 2.492337 -0.827820 0.071900
 C4 -1.797459 -0.656709 -0.324245
 N5 2.475072 0.519770 0.113630
 N6 -1.215554 0.563605 -0.172842
 N7 -0.949432 -1.675251 -0.294055
 N8 1.484309 -1.699265 -0.057522

C9 0.284054 -1.078426 -0.129460
 N10 3.766483 -1.397515 0.215977
 H11 3.831567 -2.323015 -0.191173
 H12 4.507855 -0.768363 -0.068118
 O13 1.208856 2.450420 0.047191
 H14 -3.222096 -2.273963 0.737736
 H15 -1.646946 1.493560 -0.154727
 O16 -3.130575 -0.782843 -0.475925
 O17 -3.695810 -1.418576 0.783994
 O18 -1.272136 3.394039 -0.013807
 H19 -0.294404 3.128547 -0.019177
 H20 -1.415921 3.802340 0.851974

Zero-point correction= 0.135262 (Hartree/Particle)
 Thermal correction to Energy= 0.148277
 Thermal correction to Enthalpy= 0.149221
 Thermal correction to Gibbs Free Energy= 0.095163
 Sum of electronic and zero-point Energies= -768.709211
 Sum of electronic and thermal Energies= -768.696196
 Sum of electronic and thermal Enthalpies= -768.695251
 Sum of electronic and thermal Free Energies= -768.749310

TS2c⁻(H₂O)

C1 -1.124834 1.271981 0.041109
 C2 -0.072368 0.251712 -0.063321
 C3 -2.573516 -0.576243 0.105963
 C4 1.669526 -0.981349 -0.465051
 N5 -2.385945 0.754211 0.157796
 N6 1.268044 0.388588 -0.193711
 N7 0.681928 -1.886477 -0.387327
 N8 -1.693109 -1.580650 -0.073964
 C9 -0.428536 -1.133163 -0.159634
 N10 -3.889465 -0.981648 0.285263
 H11 -4.098852 -1.902635 -0.077715
 H12 -4.574802 -0.262209 0.095099
 O13 -0.896505 2.500288 0.029654
 H14 1.633581 -0.025550 -1.387842
 O15 3.387046 -1.349809 1.033326
 O16 2.999323 -1.273698 -0.407063
 H17 3.491138 -0.397051 1.224710
 O18 1.755898 3.480197 -0.034180
 H19 2.104349 2.576060 -0.095173
 H20 0.786690 3.299739 -0.003759

Zero-point correction= 0.129651 (Hartree/Particle)
 Thermal correction to Energy= 0.142782
 Thermal correction to Enthalpy= 0.143726
 Thermal correction to Gibbs Free Energy= 0.089238
 Sum of electronic and zero-point Energies= -768.623822
 Sum of electronic and thermal Energies= -768.610691
 Sum of electronic and thermal Enthalpies= -768.609746
 Sum of electronic and thermal Free Energies= -768.664234

TS2c⁻_1(H₂O)

C1 -1.115033 1.450050 -0.191679
 C2 -0.138224 0.325428 -0.390673
 C3 -2.637622 -0.293262 0.196055
 C4 1.594619 -1.094510 -0.722573
 N5 -2.372625 1.037860 0.084392

N6 1.107341 0.341923 -0.697673
 N7 0.452945 -1.896218 -0.321408
 N8 -1.852462 -1.373696 0.088434
 C9 -0.562482 -1.087419 -0.196932
 N10 -3.963481 -0.563253 0.443258
 H11 -4.170913 -1.489040 0.792011
 H12 -4.513933 0.208949 0.792048
 O13 -0.734748 2.624006 -0.294101
 H14 1.813301 -1.331481 -1.777725
 H15 1.817255 1.135835 -0.549356
 O16 2.790639 -1.224835 -0.067933
 O17 2.698960 -0.584166 1.260065
 O18 3.094370 1.662428 0.306108
 H19 3.023205 0.678709 0.848730
 H20 2.787749 2.349544 0.916973

Zero-point correction= 0.130980 (Hartree/Particle)
 Thermal correction to Energy= 0.142676
 Thermal correction to Enthalpy= 0.143620
 Thermal correction to Gibbs Free Energy= 0.092870
 Sum of electronic and zero-point Energies= -768.643776
 Sum of electronic and thermal Energies= -768.632080
 Sum of electronic and thermal Enthalpies= -768.631136
 Sum of electronic and thermal Free Energies= -768.681886

8-OOH[G - 2H]⁻_1(H₂O)

C1 -1.034395 1.414442 -0.275640
 C2 -0.087974 0.266474 -0.496706
 C3 -2.587645 -0.270569 0.214559
 C4 1.557534 -1.143597 -0.780547
 N5 -2.301649 1.044893 0.042375
 N6 1.142008 0.285211 -0.856138
 N7 0.458778 -1.956214 -0.306213
 N8 -1.821724 -1.373898 0.166870
 C9 -0.540365 -1.124418 -0.181715
 N10 -3.919765 -0.511166 0.481858
 H11 -4.125583 -1.411864 0.892679
 H12 -4.445631 0.285081 0.815093
 O13 -0.636185 2.586403 -0.355368
 H14 1.854597 -1.465305 -1.790286
 H15 2.297247 1.634595 -0.250122
 O16 2.778847 -1.263179 -0.072161
 O17 2.609980 -0.746101 1.279458
 O18 2.830187 2.028919 0.485222
 H19 2.818639 0.211262 1.142144
 H20 2.191631 2.622123 0.912323

Zero-point correction= 0.135804 (Hartree/Particle)
 Thermal correction to Energy= 0.148587
 Thermal correction to Enthalpy= 0.149531
 Thermal correction to Gibbs Free Energy= 0.096145
 Sum of electronic and zero-point Energies= -768.677079
 Sum of electronic and thermal Energies= -768.664296
 Sum of electronic and thermal Enthalpies= -768.663352
 Sum of electronic and thermal Free Energies= -768.716738

**Cartesian coordinates for the structures in Fig. 6,
optimized at B3LYP/6-31+G***

8-oxo[G – 3H]⁻ + H₂O

C1 -0.903509 1.486619 -0.002758
 C2 0.093533 0.355410 -0.004820
 C3 -2.509908 -0.212155 -0.003808
 C4 1.719698 -1.096718 -0.000542
 N5 -2.217024 1.091832 -0.000687
 N6 1.371982 0.371437 -0.003685
 N7 0.604339 -1.909783 -0.000462
 N8 -1.716424 -1.333415 -0.004143
 C9 -0.420548 -1.065756 -0.003720
 N10 -3.841438 -0.508385 -0.026929
 H11 -4.117930 -1.465599 0.134718
 H12 -4.496639 0.243574 0.128292
 O13 -0.544928 2.663562 0.000399
 H14 4.139045 0.166810 0.005331
 H15 3.476228 1.512875 0.002621
 O16 2.893550 -1.436870 0.002436
 O17 4.365586 1.117824 0.006449

Zero-point correction=	0.107718 (Hartree/Particle)
Thermal correction to Energy=	0.119797
Thermal correction to Enthalpy=	0.120741
Thermal correction to Gibbs Free Energy=	0.068450
Sum of electronic and zero-point Energies=	-692.382878
Sum of electronic and thermal Energies=	-692.370799
Sum of electronic and thermal Enthalpies=	-692.369855
Sum of electronic and thermal Free Energies=	-692.422146

TS3a⁻

C1 -0.829097 1.281506 -0.482772
 C2 0.335053 0.369165 -0.241267
 C3 -2.102709 -0.584074 0.092971
 C4 2.236692 -0.814282 -0.201166
 N5 -2.045857 0.714415 -0.200068
 N6 1.620379 0.536616 -0.397273
 N7 1.248168 -1.759454 -0.049770
 N8 -1.131025 -1.557646 0.122230
 C9 0.095571 -1.092094 -0.043437
 N10 -3.340547 -1.064986 0.410937
 H11 -3.461239 -2.066092 0.456176
 H12 -4.135950 -0.466534 0.243479
 O13 -0.684799 2.394456 -0.986020
 H14 1.953468 1.397706 0.145562
 H15 1.065922 2.577012 2.080475
 O16 1.204589 1.743877 1.597370
 O17 3.443574 -0.949086 -0.220608

Zero-point correction=	0.104935 (Hartree/Particle)
Thermal correction to Energy=	0.116027
Thermal correction to Enthalpy=	0.116972
Thermal correction to Gibbs Free Energy=	0.068021
Sum of electronic and zero-point Energies=	-692.310839
Sum of electronic and thermal Energies=	-692.299746
Sum of electronic and thermal Enthalpies=	-692.298802
Sum of electronic and thermal Free Energies=	-692.347753

5-OH-8-oxo[G – 2H]⁻

C1 -0.803516 1.317986 -0.348620
 C2 0.378218 0.552269 0.275713
 C3 -1.987957 -0.656897 -0.097209
 C4 2.339934 -0.530836 -0.241126
 N5 -1.981696 0.652042 -0.425225
 N6 1.685626 0.720205 -0.282778
 N7 1.392458 -1.557242 -0.088010
 N8 -0.975384 -1.526223 0.107833
 C9 0.236186 -0.963030 0.106354
 N10 -3.242458 -1.213893 -0.004695
 H11 -3.281176 -2.222032 -0.071214
 H12 -3.987322 -0.685571 -0.438249
 O13 -0.652807 2.519649 -0.614099
 H14 2.226372 1.551233 -0.081098
 H15 0.105439 1.806061 1.753051
 O16 0.330081 0.861381 1.689766
 O17 3.548936 -0.667387 -0.386045

Zero-point correction=	0.111618 (Hartree/Particle)
Thermal correction to Energy=	0.121771
Thermal correction to Enthalpy=	0.122716
Thermal correction to Gibbs Free Energy=	0.076021
Sum of electronic and zero-point Energies=	-692.388522
Sum of electronic and thermal Energies=	-692.378369
Sum of electronic and thermal Enthalpies=	-692.377425
Sum of electronic and thermal Free Energies=	-692.424119

TS3b⁻

C1 -0.676141 1.289846 -0.399646
 C2 0.404502 0.577181 0.428260
 C3 -1.966691 -0.624243 -0.041298
 C4 2.409085 -0.433297 -0.140440
 N5 -1.914173 0.758876 0.189251
 N6 1.796561 0.796163 0.128633
 N7 1.423866 -1.435061 -0.369194
 N8 -0.952976 -1.452129 -0.233821
 C9 0.279659 -0.884190 -0.086930
 N10 -3.225619 -1.150333 -0.009025
 H11 -3.326132 -2.111891 -0.305034
 H12 -3.991325 -0.511376 -0.167096
 O13 -0.631054 2.115671 -1.275944
 H14 2.310479 1.460506 0.693292
 H15 -1.377631 0.800575 1.245581
 O16 -0.014541 0.764172 1.735352
 O17 3.619160 -0.606369 -0.205325

Zero-point correction=	0.106959 (Hartree/Particle)
Thermal correction to Energy=	0.116663
Thermal correction to Enthalpy=	0.117607
Thermal correction to Gibbs Free Energy=	0.071692
Sum of electronic and zero-point Energies=	-692.334915
Sum of electronic and thermal Energies=	-692.325211
Sum of electronic and thermal Enthalpies=	-692.324267
Sum of electronic and thermal Free Energies=	-692.370182

5-O-8-oxo[G - 2H]⁻

C1 -0.667831 1.361903 -0.307259
 C2 0.424622 0.579931 0.440329

C3 -1.959700 -0.727358 -0.070282
 C4 2.390679 -0.484736 -0.234325
 N5 -1.880348 0.618113 -0.360302
 N6 1.793725 0.759289 -0.090020
 N7 1.391723 -1.513804 -0.226924
 N8 -0.949833 -1.530140 0.092433
 C9 0.282609 -0.919650 0.081927
 N10 -3.246427 -1.239922 0.022185
 H11 -3.246520 -2.253224 -0.005304
 H12 -3.945160 -0.823609 -0.582478
 O13 -0.674412 2.525595 -0.678004
 H14 2.351413 1.492735 0.331611
 H15 -2.725239 1.169083 -0.470715
 O16 0.207455 0.902075 1.715707
 O17 3.589626 -0.690205 -0.387335

Zero-point correction= 0.110980 (Hartree/Particle)
 Thermal correction to Energy= 0.121266
 Thermal correction to Enthalpy= 0.122210
 Thermal correction to Gibbs Free Energy= 0.075310
 Sum of electronic and zero-point Energies= -692.359358
 Sum of electronic and thermal Energies= -692.349072
 Sum of electronic and thermal Enthalpies= -692.348128
 Sum of electronic and thermal Free Energies= -692.395028

TS3c⁻

C1 0.613437 0.340199 0.926788
 C2 0.274354 -0.847751 0.056793
 C3 -1.993693 -0.649133 -0.107001
 C4 -0.666056 1.331019 -0.538431
 C5 2.390233 -0.469844 -0.308111
 N6 -1.932982 0.693391 -0.410967
 N7 -0.972801 -1.419188 0.066011
 O8 -0.628845 2.476165 -0.952686
 N9 1.306548 -1.307536 -0.619468
 N10 -3.282751 -1.192623 -0.093146
 H11 -3.957874 -0.636273 0.421199
 H12 -3.255793 -2.149951 0.244377
 O13 3.542480 -0.579221 -0.723262
 N14 1.953772 0.548415 0.543309
 O15 0.108213 0.725094 1.997928

H16 2.578406 1.188037 1.011906
 H17 -2.751676 1.137721 -0.833718

Zero-point correction= 0.108426 (Hartree/Particle)
 Thermal correction to Energy= 0.118881
 Thermal correction to Enthalpy= 0.119825
 Thermal correction to Gibbs Free Energy= 0.072176
 Sum of electronic and zero-point Energies= -692.342633
 Sum of electronic and thermal Energies= -692.332178
 Sum of electronic and thermal Enthalpies= -692.331234
 Sum of electronic and thermal Free Energies= -692.378884

[Sp - H]⁻

C1 0.892825 0.317400 1.173018
 C2 0.073878 -0.114135 -0.088346
 C3 -2.091407 -0.614054 -0.004302
 C4 -0.747473 1.092561 -0.631381
 C5 2.227052 -0.556101 -0.535883
 N6 -2.068048 0.640169 -0.636671
 N7 -0.958768 -1.109605 0.309482
 O8 -0.385533 2.197406 -0.982552
 N9 1.007541 -0.612701 -1.059965
 N10 -3.336369 -1.195552 0.242962
 H11 -3.955960 -1.178579 -0.563540
 H12 -3.211356 -2.145880 0.580453
 O13 3.337981 -0.877725 -0.982129
 N14 2.155627 0.004438 0.829390
 O15 0.462727 0.813254 2.212818
 H16 2.969179 0.142590 1.413258
 H17 -2.852402 1.277123 -0.690283

Zero-point correction= 0.110664 (Hartree/Particle)
 Thermal correction to Energy= 0.121310
 Thermal correction to Enthalpy= 0.122254
 Thermal correction to Gibbs Free Energy= 0.073892
 Sum of electronic and zero-point Energies= -692.383476
 Sum of electronic and thermal Energies= -692.372830
 Sum of electronic and thermal Enthalpies= -692.371886
 Sum of electronic and thermal Free Energies= -692.420248

Comparison of critical energetics in Figs. 2-3 at B3LYP/6-31+G* and wB97xD/6-31+G*

	B3LYP/6-31+G* (eV)	wB97xD/6-31+G* (eV)
PC ⁺	0.07	-0.08
TS1a ⁺	-0.02	0.08
TS2a ⁺	0.78	1.23
5,8-OO-[G + H] ⁺	-0.81	-1.00
8-OO[G + H] ⁺	0.67	0.88
PC ⁻	-0.82	-0.67
TS1 ⁻	-0.82	-0.70
TS2a ⁻	-0.34	0.04
5,8-OO-[G - H] ⁻	-1.45	-1.65
8-OO[G - H] ⁻	-0.71	-0.62

All energetics calculated using two different functionals are in reasonable agreement, except those of TS2a⁺ and TS2a⁻. The latter correspond to the barriers for formation of 8-OO[G - H]⁺ and 8-OO[G - H]⁻ from corresponding reactants, respectively. However, both B3LYP and wB97xD calculations indicate these routes are much less favorable than direct 5,8-OO[G + H]⁺ → 8-OO[G + H]⁺ and 5,8-OO[G - H]⁻ → 8-OO[G - H]⁻. Therefore, the problematic TS2a⁺ and TS2a⁻ are mechanistically insignificant, and would not affect the reactions.

Cartesian coordinates for the critical structures optimized at wB97xD/6-31+G*

[G + H]⁺		H3 -2.648911 1.371054 0.367186	
C1 0.254908 1.466876 -0.000001		C4 -2.024966 -0.585671 0.039293	
C2 -0.785040 0.471972 -0.000002		H5 1.446730 -2.395351 -0.994846	
H3 2.300711 1.453482 0.000000		C6 2.231284 -0.449957 -1.083966	
C4 1.719738 -0.544089 0.000004		N7 -1.865974 0.780136 0.105539	
H5 -1.800999 -2.541815 0.000000		N8 1.674386 0.738820 -0.878986	
C6 -2.686347 -0.636945 -0.000004		N9 1.293024 -1.396210 -0.917826	
N7 1.510000 0.816893 0.000002		N10 -1.048923 -1.419325 -0.297477	
N8 -2.161053 0.579156 -0.000004		C11 0.100561 -0.800542 -0.552732	
N9 -1.687793 -1.534430 -0.000001		N12 -3.227962 -1.089591 0.329429	
N10 0.736397 -1.431856 0.000004		H13 -3.346083 -2.092430 0.288571	
C11 -0.473453 -0.868382 0.000000		H14 -4.020466 -0.525465 0.596406	
N12 2.985041 -0.979689 0.000005		O15 -0.612012 2.700226 -0.119285	
H13 3.145205 -1.977209 0.000010		H16 3.259409 -0.626290 -1.361806	
H14 3.786095 -0.367012 0.000015		H17 2.156324 1.631186 -0.916502	
O15 0.141857 2.670727 -0.000003		O18 1.303487 -0.214415 1.899706	
H16 -3.740556 -0.869862 -0.000006		O19 2.490666 -0.231992 1.644956	
H17 -2.682289 1.449482 -0.000006			
Zero-point correction=	0.132322 (Hartree/Particle)	Zero-point correction=	0.137422 (Hartree/Particle)
Thermal correction to Energy=	0.140711	Thermal correction to Energy=	0.149347
Thermal correction to Enthalpy=	0.141655	Thermal correction to Enthalpy=	0.150291
Thermal correction to Gibbs Free Energy=	0.099130	Thermal correction to Gibbs Free Energy=	0.098611
Sum of electronic and zero-point Energies=	-542.643814	Sum of electronic and zero-point Energies=	-692.858994
Sum of electronic and thermal Energies=	-542.635425	Sum of electronic and thermal Energies=	-692.847069
Sum of electronic and thermal Enthalpies=	-542.634481	Sum of electronic and thermal Enthalpies=	-692.846124
Sum of electronic and thermal Free Energies=	-542.677006	Sum of electronic and thermal Free Energies=	-692.897805
PC⁺		TS1a⁺	
C1 -0.680214 1.495899 -0.175958		C1 -0.661779 1.496252 -0.148321	
C2 0.360671 0.558591 -0.521099		C2 0.432321 0.558095 -0.368362	
		H3 -2.658445 1.370165 0.279974	

C4 -2.003023 -0.584182 -0.004669
 H5 1.538499 -2.414183 -0.684935
 C6 2.326936 -0.459359 -0.656669
 N7 -1.855129 0.782318 0.079278
 N8 1.709151 0.752919 -0.756313
 N9 1.357436 -1.418545 -0.741829
 N10 -1.006943 -1.427042 -0.283640
 C11 0.162699 -0.839555 -0.441557
 N12 -3.211885 -1.094180 0.204367
 H13 -3.317704 -2.099399 0.157652
 H14 -4.023678 -0.538821 0.433168
 O15 -0.600338 2.697528 -0.147357
 H16 3.365109 -0.630791 -0.899010
 H17 2.199289 1.637267 -0.663897
 O18 1.077425 -0.158598 1.545948
 O19 2.323613 -0.228934 1.299094

Zero-point correction= 0.138053 (Hartree/Particle)
 Thermal correction to Energy= 0.148208
 Thermal correction to Enthalpy= 0.149152
 Thermal correction to Gibbs Free Energy= 0.102558
 Sum of electronic and zero-point Energies= -692.851196
 Sum of electronic and thermal Energies= -692.841041
 Sum of electronic and thermal Enthalpies= -692.840097
 Sum of electronic and thermal Free Energies= -692.886691

TS2a⁺

C1 -0.912737 1.480852 -0.106958
 C2 0.157391 0.523184 -0.310202
 C3 -2.285333 -0.555243 0.183428
 C4 2.077384 -0.558502 -0.598398
 N5 -2.122135 0.805886 0.169147
 N6 1.440674 0.709005 -0.637396
 N7 1.026363 -1.492759 -0.656351
 N8 -1.297058 -1.423265 -0.064785
 C9 -0.124418 -0.870181 -0.298656
 N10 -3.488863 -1.047935 0.454968
 H11 -3.599892 -2.053879 0.464420
 H12 -4.295625 -0.476487 0.662317
 O13 -0.826298 2.683696 -0.144295
 H14 2.895537 -0.710526 -1.299439
 H15 1.947088 1.587887 -0.611747
 O16 2.728659 -0.651952 0.794745
 O17 3.399080 0.437069 0.977965
 H18 -2.910553 1.420759 0.348004
 H19 1.165328 -2.495457 -0.665236

Zero-point correction= 0.136351 (Hartree/Particle)
 Thermal correction to Energy= 0.146910
 Thermal correction to Enthalpy= 0.147854
 Thermal correction to Gibbs Free Energy= 0.099833
 Sum of electronic and zero-point Energies= -692.809419
 Sum of electronic and thermal Energies= -692.798860
 Sum of electronic and thermal Enthalpies= -692.797915
 Sum of electronic and thermal Free Energies= -692.845936

5,8-OO-[G + H]⁺

C1 -0.594961 1.451073 -0.134929
 C2 0.547306 0.465039 -0.081076

H3 -2.632062 1.454889 0.040019
 C4 -2.049815 -0.539351 0.030377
 H5 1.410315 -2.609707 -0.406920
 C6 2.307113 -0.581833 -0.360407
 N7 -1.841266 0.817572 0.006450
 N8 1.645093 0.546319 -0.993613
 N9 1.264488 -1.609540 -0.482443
 N10 -1.083544 -1.462182 -0.122754
 C11 0.121170 -0.978516 -0.263250
 N12 -3.283538 -0.979519 0.198676
 H13 -3.433560 -1.981651 0.203328
 H14 -4.082844 -0.376339 0.339796
 O15 -0.479583 2.634223 -0.261618
 H16 3.290813 -0.866838 -0.722630
 H17 2.171419 1.413285 -0.881740
 O18 1.132313 0.454482 1.247831
 O19 2.395072 -0.228786 1.018743

Zero-point correction= 0.141269 (Hartree/Particle)
 Thermal correction to Energy= 0.150608
 Thermal correction to Enthalpy= 0.151552
 Thermal correction to Gibbs Free Energy= 0.106656
 Sum of electronic and zero-point Energies= -692.891551
 Sum of electronic and thermal Energies= -692.882212
 Sum of electronic and thermal Enthalpies= -692.881268
 Sum of electronic and thermal Free Energies= -692.926164

8-OO[G + H]⁺

C1 -0.903716 1.465789 -0.144598
 C2 0.187183 0.528345 -0.313703
 C3 -2.234714 -0.598158 0.112428
 C4 2.235296 -0.551810 -0.606724
 N5 -2.118618 0.763846 0.042071
 N6 1.488741 0.743526 -0.352936
 N7 1.142794 -1.500606 -0.358648
 N8 -1.205077 -1.452984 -0.019118
 C9 -0.033837 -0.889457 -0.208842
 N10 -3.433505 -1.123161 0.317462
 H11 -3.507504 -2.131473 0.372896
 H12 -4.274383 -0.575005 0.435305
 O13 -0.845895 2.668782 -0.157134
 H14 2.651986 -0.679195 -1.611393
 H15 1.905539 1.646932 -0.581790
 O16 3.197135 -0.430989 0.334167
 O17 2.431422 0.404923 1.218647
 H18 -2.933134 1.358640 0.161961
 H19 1.274575 -2.504213 -0.375614

Zero-point correction= 0.139220 (Hartree/Particle)
 Thermal correction to Energy= 0.149550
 Thermal correction to Enthalpy= 0.150494
 Thermal correction to Gibbs Free Energy= 0.103176
 Sum of electronic and zero-point Energies= -692.821798
 Sum of electronic and thermal Energies= -692.811467
 Sum of electronic and thermal Enthalpies= -692.810523
 Sum of electronic and thermal Free Energies= -692.857842

PC⁻

C1 -0.262817 1.424894 -0.003488

C2 0.764460 0.415716 -0.011521
 C3 -1.687954 -0.436387 -0.019135
 C4 2.607538 -0.768466 0.010900
 N5 -1.526671 0.896864 -0.009365
 N6 2.140495 0.508366 0.001225
 N7 1.652491 -1.675512 0.007065
 N8 -0.788388 -1.421082 -0.009897
 C9 0.478371 -0.937971 -0.006558
 N10 -3.028503 -0.854491 -0.072496
 H11 -3.155444 -1.775621 0.325963
 H12 -3.652874 -0.157920 0.312307
 O13 -0.008203 2.648292 0.012758
 H14 3.668142 -0.988674 0.019658
 H15 2.662247 1.370143 0.003111

Zero-point correction= 0.105528 (Hartree/Particle)
 Thermal correction to Energy= 0.113371
 Thermal correction to Enthalpy= 0.114315
 Thermal correction to Gibbs Free Energy= 0.072774
 Sum of electronic and zero-point Energies= -541.745876
 Sum of electronic and thermal Energies= -541.738032
 Sum of electronic and thermal Enthalpies= -541.737088
 Sum of electronic and thermal Free Energies= -541.778629

TS1⁻

C1 -0.643253 1.436577 -0.223216
 C2 0.430436 0.451247 -0.364709
 C3 -1.986617 -0.458466 0.015337
 C4 2.203976 -0.697815 -0.829481
 N5 -1.861665 0.873828 0.033715
 N6 1.703328 0.585636 -0.835901
 N7 1.279057 -1.635099 -0.732997
 N8 -1.084802 -1.432694 -0.229412
 C9 0.138010 -0.943125 -0.436155
 N10 -3.270493 -0.921335 0.246391
 H11 -3.311164 -1.875471 0.574840
 H12 -3.860520 -0.261617 0.732656
 O13 -0.434140 2.650400 -0.325163
 H14 3.244908 -0.891695 -1.050045
 H15 2.260635 1.396238 -0.605142
 O16 2.306756 -0.165652 1.480790
 O17 1.058990 0.091462 1.594929

Zero-point correction= 0.111435 (Hartree/Particle)
 Thermal correction to Energy= 0.122091
 Thermal correction to Enthalpy= 0.123035
 Thermal correction to Gibbs Free Energy= 0.074854
 Sum of electronic and zero-point Energies= -691.981910
 Sum of electronic and thermal Energies= -691.971254
 Sum of electronic and thermal Enthalpies= -691.970309
 Sum of electronic and thermal Free Energies= -692.018490

TS2a⁻

C1 -0.982095 1.449934 -0.075217
 C2 0.057693 0.447876 -0.352201
 C3 -2.341670 -0.439651 0.166086
 C4 1.900488 -0.727547 -0.619894
 N5 -2.200031 0.902346 0.168735
 N6 1.348141 0.568585 -0.612815

N7 0.909621 -1.652328 -0.494458
 N8 -1.452153 -1.421538 -0.027240
 C9 -0.215565 -0.957445 -0.288684
 N10 -3.638231 -0.865875 0.380878
 H11 -3.718989 -1.818810 0.704692
 H12 -4.230359 -0.185608 0.834547
 O13 -0.723137 2.659851 -0.093289
 H14 2.756732 -0.924107 -1.250054
 H15 1.896633 1.412427 -0.488038
 O16 2.890581 -0.506185 0.873156
 O17 3.833986 0.366180 0.634210

Zero-point correction= 0.110359 (Hartree/Particle)
 Thermal correction to Energy= 0.120488
 Thermal correction to Enthalpy= 0.121432
 Thermal correction to Gibbs Free Energy= 0.073950
 Sum of electronic and zero-point Energies= -691.955300
 Sum of electronic and thermal Energies= -691.945172
 Sum of electronic and thermal Enthalpies= -691.944228
 Sum of electronic and thermal Free Energies= -691.991710

5,8-OO-[G - H]⁻

C1 -0.638538 1.417236 -0.128066
 C2 0.511801 0.420173 -0.078031
 C3 -2.016182 -0.457858 0.014106
 C4 2.220721 -0.687011 -0.398642
 N5 -1.874533 0.883669 -0.007849
 N6 1.612338 0.500638 -1.005121
 N7 1.221287 -1.725703 -0.472637
 N8 -1.134693 -1.459323 -0.125943
 C9 0.133299 -1.038466 -0.258603
 N10 -3.319469 -0.868693 0.162235
 H11 -3.442597 -1.824141 0.461911
 H12 -3.952087 -0.174015 0.529420
 O13 -0.391507 2.614394 -0.259549
 H14 3.212656 -0.958262 -0.757597
 H15 2.153939 1.341816 -0.806785
 O16 2.386413 -0.282617 0.998150
 O17 1.158466 0.465229 1.238108

Zero-point correction= 0.114648 (Hartree/Particle)
 Thermal correction to Energy= 0.123573
 Thermal correction to Enthalpy= 0.124517
 Thermal correction to Gibbs Free Energy= 0.080367
 Sum of electronic and zero-point Energies= -692.015887
 Sum of electronic and thermal Energies= -692.006961
 Sum of electronic and thermal Enthalpies= -692.006017
 Sum of electronic and thermal Free Energies= -692.050167

8-OO[G - H]⁻

C1 1.065630 1.466020 0.008813
 C2 -0.075537 0.499027 0.145910
 C3 2.351826 -0.488571 -0.061941
 C4 -2.013317 -0.659453 0.354312
 N5 2.267123 0.869260 -0.087721
 N6 -1.331332 0.679774 0.254535
 N7 -0.959020 -1.622724 0.199562
 N8 1.421716 -1.441219 0.036250
 C9 0.160970 -0.968487 0.135339

N10 3.638755 -0.944984 -0.129247
H11 3.761299 -1.920903 -0.351600
H12 4.333578 -0.285106 -0.442270
O13 0.837217 2.675184 0.004100
H14 -2.414813 -0.692039 1.384696
H15 -1.942295 1.493762 0.161486
O16 -3.001181 -0.696387 -0.570074
O17 -3.828022 0.462743 -0.204097

Zero-point correction= 0.111211 (Hartree/Particle)
Thermal correction to Energy= 0.121434
Thermal correction to Enthalpy= 0.122378
Thermal correction to Gibbs Free Energy= 0.075017
Sum of electronic and zero-point Energies= -691.979479
Sum of electronic and thermal Energies= -691.969255
Sum of electronic and thermal Enthalpies= -691.968311
Sum of electronic and thermal Free Energies= -692.015672