Supporting Information

The Acidity and Proton Affinity of the Damaged Base 1,N^6-Ethenoadenine in the Gas Phase versus in Solution: Intrinsic Reactivity and Biological Implications

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Note: Structure numbers correlate to structures shown on pages S8 through S17, not to structures in paper.

Full References from Manuscript

Reference numbers refer to reference numbers in manuscript.

(57) Frisch, R. C.; Trucks, G.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; C., B. J.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; COssi, M.; Scalmani, G.; Rega, N.; Peterson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nikai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G.; Salvador, P.; Dannenberg, J. J.; Zakrewski, V. G.; Dapprich, S.; Daniels, A.; Strain, M.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavarchari, K.; Foresman, J.; Ortiz, J.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M.; Johnson, B.; Chen, W.; Wong, M.; Gonzalez, C.; Pople, J. A. GAUSSIAN03; Gaussian, Inc., Wallingford CT, 2004.

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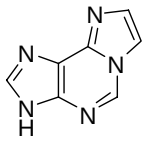
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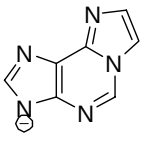
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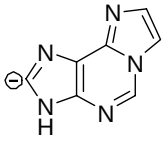
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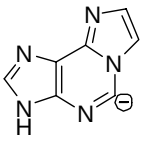
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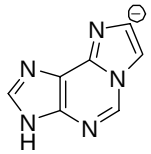
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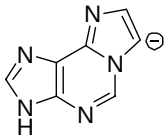
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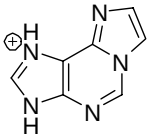
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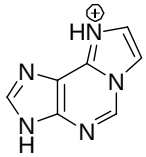
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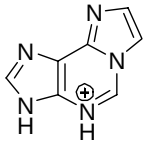
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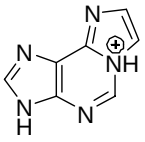
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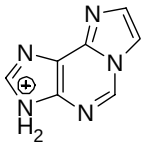
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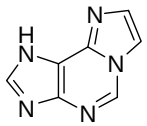
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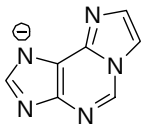
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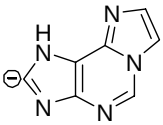
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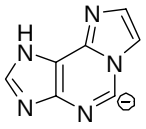
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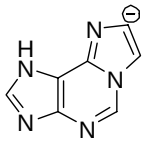
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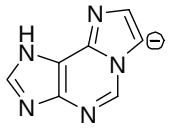
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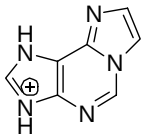
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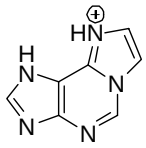
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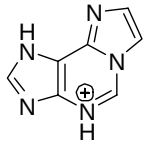
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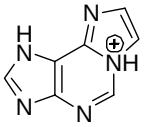
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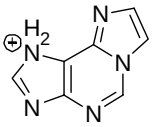
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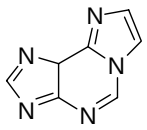

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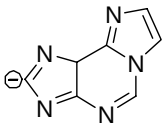

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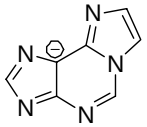

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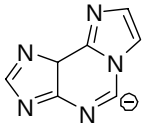

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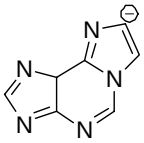

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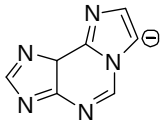

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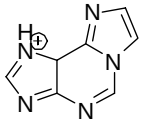

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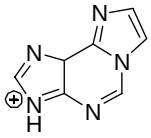

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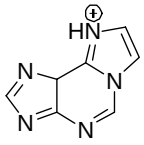

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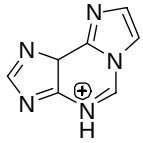

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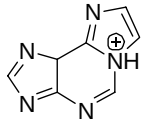

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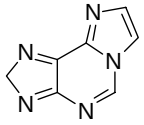

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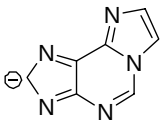

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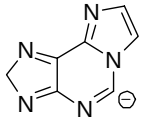

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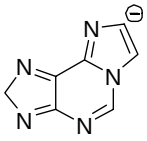

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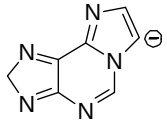

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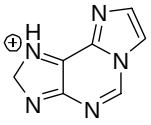

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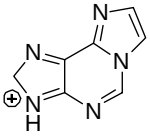

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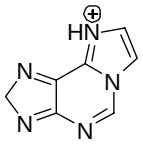

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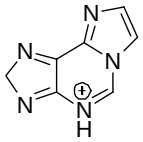

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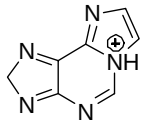

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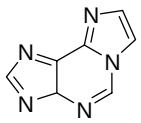

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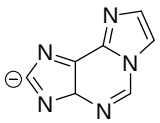

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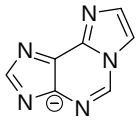

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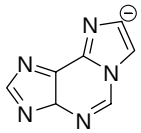

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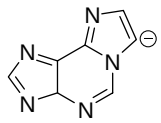

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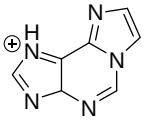

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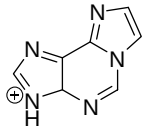

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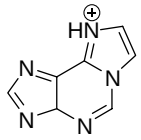

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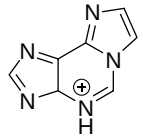

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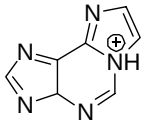

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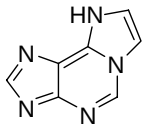
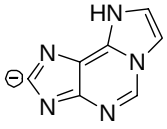
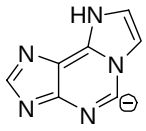


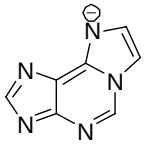
N10H



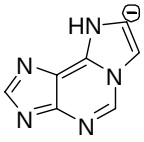
N10H C8 deprotonated



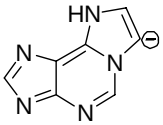
N10H C2 deprotonated



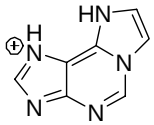
N10H N10 depronated



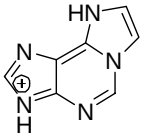
N10H C11 deprotonated



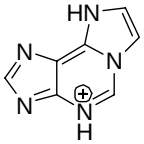
N10H C12 deprotonated



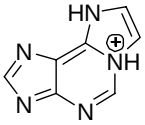
N10H N7 protonated



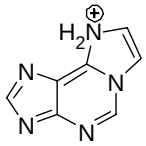
N10H N9 protonated



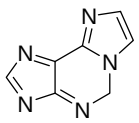
N10H N3 protonated



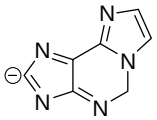
N10H N1 protonated



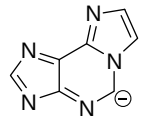
N10H N10 protonated



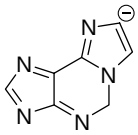
C2H



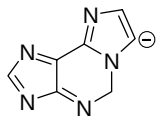
C2H C8 deprotonated



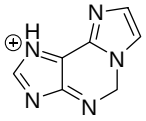
C2H C2 deprotonated



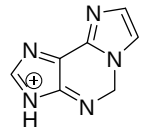
C2H C11 deprotonated



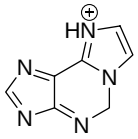
C2H C12 deprotonated



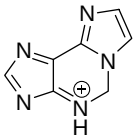
C2H N7 protonated



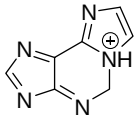
C2H N9 protonated



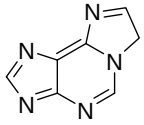
C2H N10 protonated



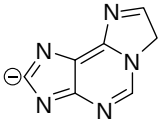
C2H N3 protonated



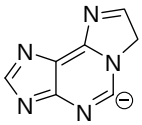
C2H N1 protonated



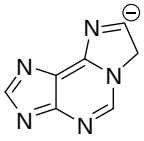
C12H



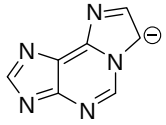
C12H C8 deprotonated



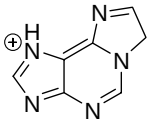
C12H C2 deprotonated



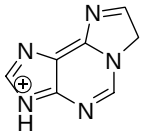
C12H C11 deprotonated



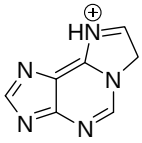
C12H C12 deprotonated



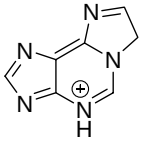
C12H N7 protonated



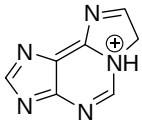
C12H N9 protonated



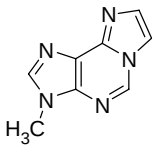
C12H N10 protonated



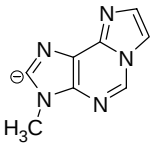
C12H N3 protonated



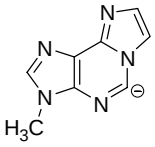
C12H N1 protonated



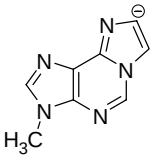
N9CH3



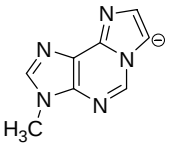
N9CH3 C8 deprotonated



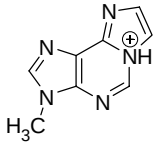
N9CH3 C2 deprotonated



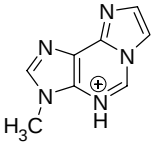
N9CH3 C11 protonated



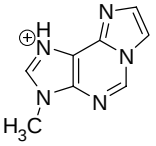
N9CH3 C12 deprotonated



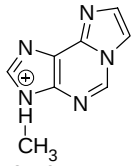
N9CH3 N1 protonated



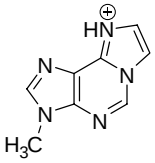
N9CH3 N3 prtonated



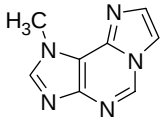
N9CH3 N7 protonated



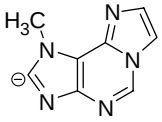
N9CH3 N9 protonated



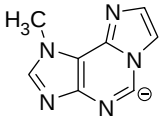
N9CH3 N10 protonated



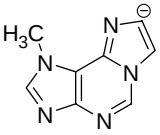
N7CH3



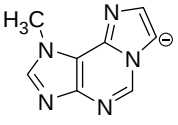
N7CH3 C8 deprotonated



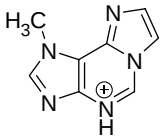
N7CH3 C2 deprotonated



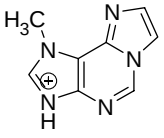
N7CH3 C11 protonated



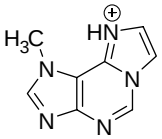
N7CH3 C12 deprotonated



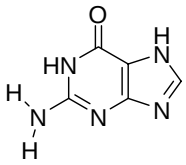
N7CH3 N3 protonated

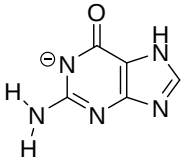


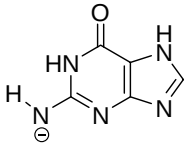
N7CH3 N9 protonated

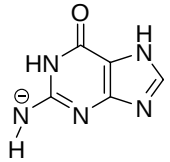


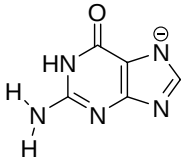
N7CH3 N10 protonated

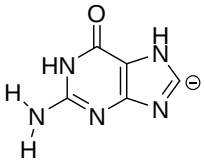

7H-keto-guanine

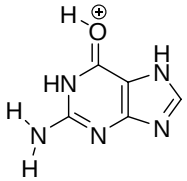

7H-keto-guanine
N1 deprotonated

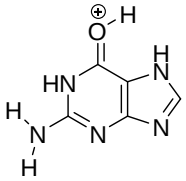

7H-keto-guanine
N2Ha deprotonated

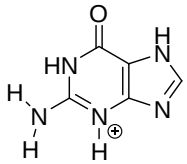

7H-keto-guanine
N2Hb deprotonated

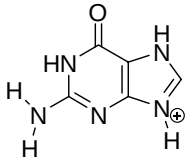

7H-keto-guanine
N7 deprotonated

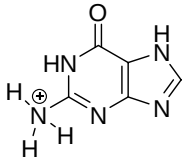

7H-keto-guanine
C8 deprotonated

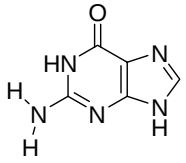

7H-keto-guanine
OHa protonated

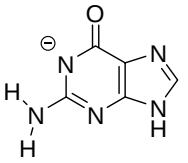

7H-keto-guanine
OHb protonated

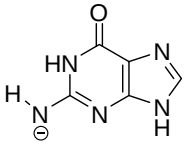

7H-keto-guanine
N3 protonated

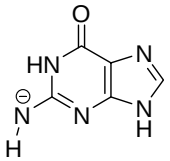

7H-keto-guanine
N9 protonated

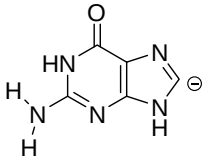

7H-keto-guanine
N2 protonated

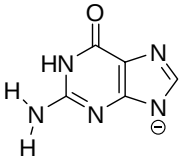

9H-keto-guanine

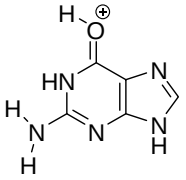

9H-keto-guanine
N1 deprotonated

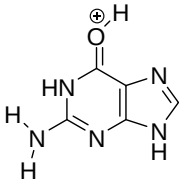

9H-keto-guanine
N2Ha deprotonated

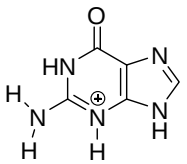

9H-keto-guanine
N2Hb deprotonated

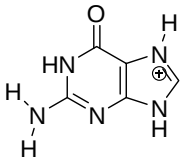

9H-keto-guanine
C8 deprotonated

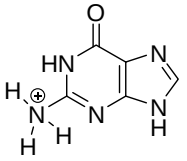

9H-keto-guanine
N9 deprotonated

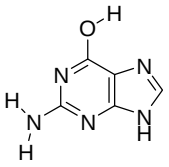

9H-keto-guanine
OHa protonated


9H-keto-guanine
OHb protonated

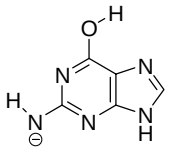

9H-keto-guanine
N3 protonated


9H-keto-guanine
N7 protonated

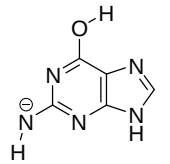

9H-keto-guanine
N2 protonated



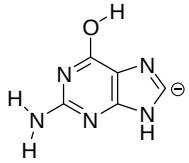
9H-trans-enol-guanine



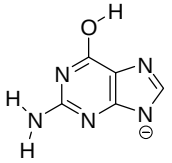
9H-trans-enol-guanine
NHa deprotonated



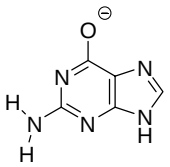
9H-trans-enol-guanine
NHb deprotonated



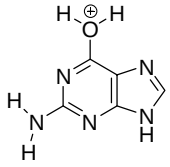
9H-trans-enol-guanine
C8 deprotonated



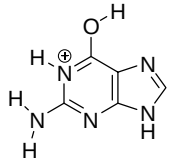
9H-trans-enol-guanine
N9 deprotonated



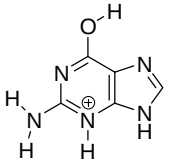
9H-trans-enol-guanine
OH deprotonated



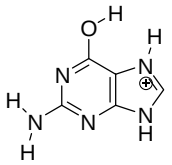
9H-trans-enol-guanine
OHa protonated



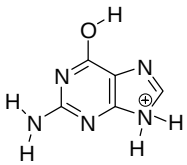
9H-trans-enol-guanine
N1 protonated



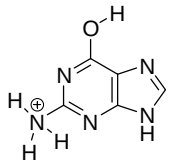
9H-trans-enol-guanine
N3 protonated



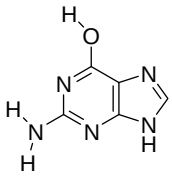
9H-trans-enol-guanine
N7 protonated



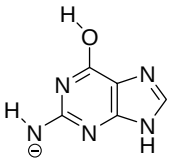
9H-trans-enol-guanine
N9H protonated



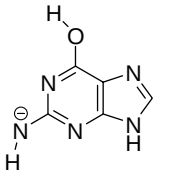
9H-trans-enol-guanine
N2 protonated



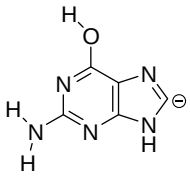
9H-cis-enol-guanine



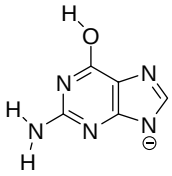
9H-cis-enol-guanine
N2Ha deprotonated



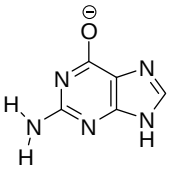
9H-cis-enol-guanine
N2Hb deprotonated



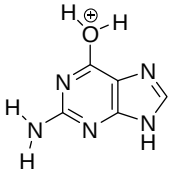
9H-cis-enol-guanine
C8 deprotonated



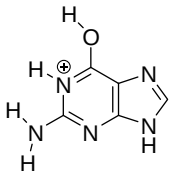
9H-cis-enol-guanine
N9 deprotonated



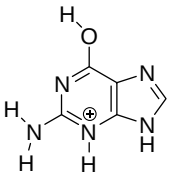
9H-cis-enol-guanine
OH deprotonated



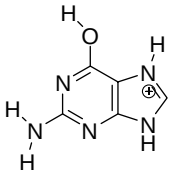
9H-cis-enol-guanine
OHb protonated



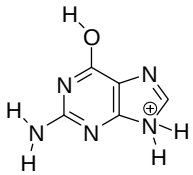
9H-cis-enol-guanine
N1 protonated



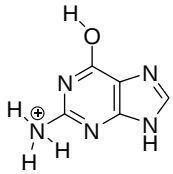
9H-cis-enol-guanine
N3 protonated



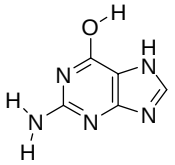
9H-cis-enol-guanine
N7 protonated

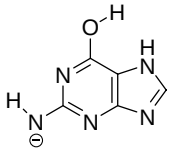


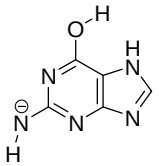
9H-cis-enol-guanine
N9H protonated

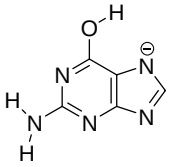


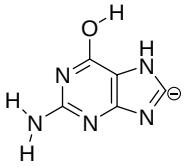
9H-cis-enol-guanine
N2 protonated

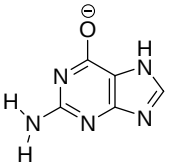

7H-trans-enol-guanine

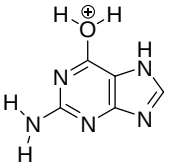

7H-trans-enol-guanine
N2Ha deprotonated

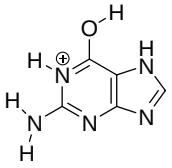

7H-trans-enol-guanine
N2Hb deprotonated

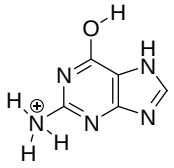

7H-trans-enol-guanine
N7 deprotonated

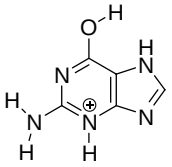

7H-trans-enol-guanine
C8 deprotonated

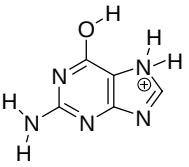

7H-trans-enol-guanine
OH deprotonated

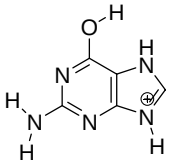

7H-trans-enol-guanine
OHa protonated

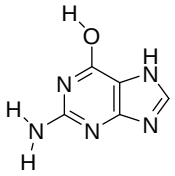

7H-trans-enol-guanine
N1 protonated

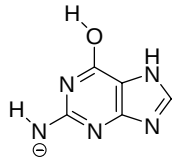

7H-trans-enol-guanine
N2 protonated

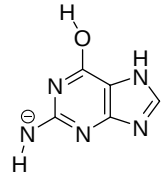

7H-trans-enol-guanine
N3 protonated

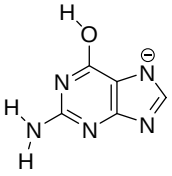

7H-trans-enol-guanine
N7H protonated

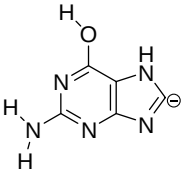

7H-trans-enol-guanine
N9 protonated

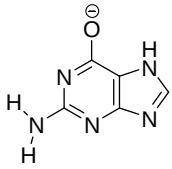

7H-cis-enol-guanine

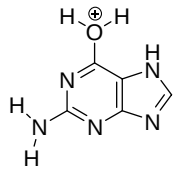

7H-cis-enol-guanine
N2Ha deprotonated

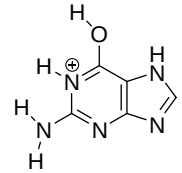

7H-cis-enol-guanine
N2Hb deprotonated

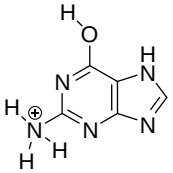

7H-cis-enol-guanine
N7 deprotonated

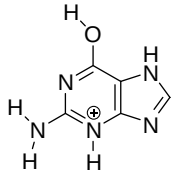

7H-cis-enol-guanine
C8 deprotonated

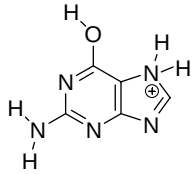

7H-cis-enol-guanine
OH deprotonated

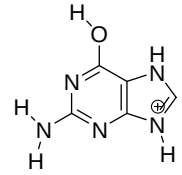

7H-cis-enol-guanine
OHb protonated

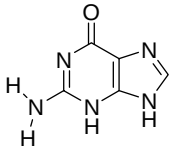

7H-cis-enol-guanine
N1 protonated

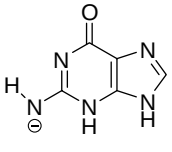

7H-cis-enol-guanine
N2 protonated

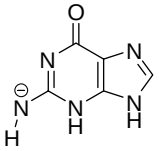

7H-cis-enol-guanine
N3 protonated

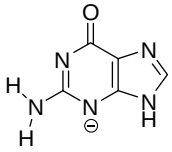

7H-cis-enol-guanine
N7H protonated

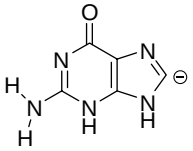

7H-cis-enol-guanine
N9 protonated

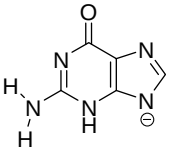

1H9H-keto-guanine

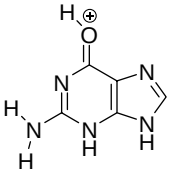

1H9H-keto-guanine
N2Ha deprotonated

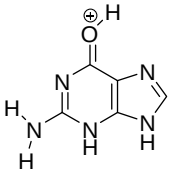

1H9H-keto-guanine
N2Hb deprotonated

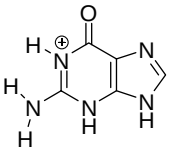

1H9H-keto-guanine
N3 deprotonated

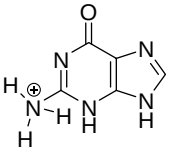

1H9H-keto-guanine
C8 deprotonated

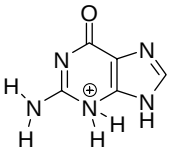

1H9H-keto-guanine
N9 deprotonated

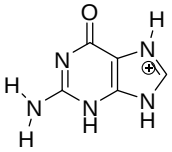

1H9H-keto-guanine
OHa protonated

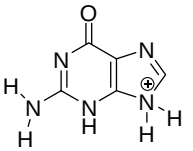

1H9H-keto-guanine
OHb protonated

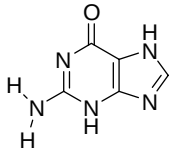

1H9H-keto-guanine
N1 protonated

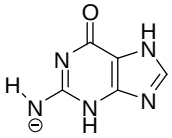

1H9H-keto-guanine
N2 protonated

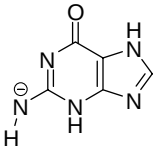

1H9H-keto-guanine
N3H protonated

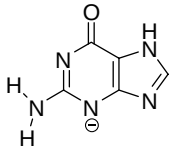

1H9H-keto-guanine
N7 protonated

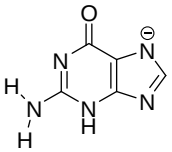

1H9H-keto-guanine
N9H protonated

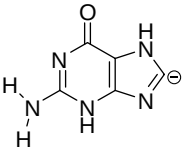

1H7H-keto-guanine

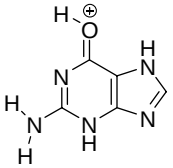

1H7H-keto-guanine
N2Ha deprotonated

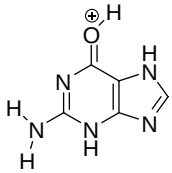

1H7H-keto-guanine
N2Hb deprotonated

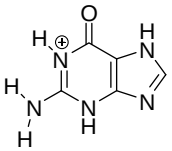

1H7H-keto-guanine
N3 deprotonated

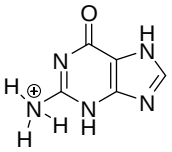

1H7H-keto-guanine
N7 deprotonated

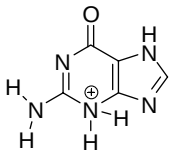

1H7H-keto-guanine
C8 deprotonated

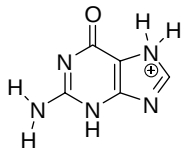

1H7H-keto-guanine
OHa protonated

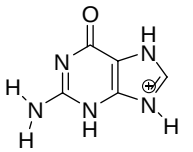

1H7H-keto-guanine
OHb protonated

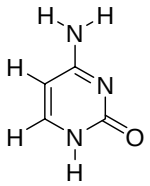

1H7H-keto-guanine
N1 protonated


1H7H-keto-guanine
N2 protonated

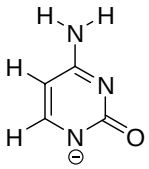

1H7H-keto-guanine
N3H protonated


1H7H-keto-guanine
N7 protonated

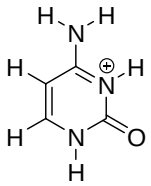

1H7H-keto-guanine
N9 protonated



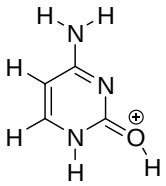
Cytosine C1



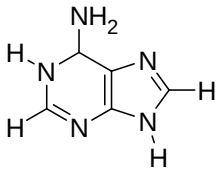
Cytosine C1
N1 deprotonated



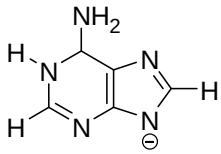
Cytosine C1
N3 protonated



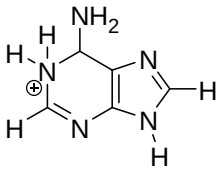
Cytosine C1
OH protonated



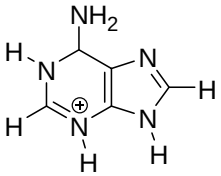
Adenine N9H amino



Adenine N9H amino
N9 deprotonated



Adenine N9H amino
N1 protonated



Adenine N9H amino
N3 protonated

1,N^6-ethenoadenine: NEUTRAL N9H
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.528564323     A.U.
 Zero-point correction=                           0.124019
(Hartree/Particle)
 Thermal correction to Energy=                    0.131621
 Thermal correction to Enthalpy=                  0.132565
 Thermal correction to Gibbs Free Energy=         0.091399
 Sum of electronic and zero-point Energies=           -543.404545
 Sum of electronic and thermal Energies=              -543.396944
 Sum of electronic and thermal Enthalpies=            -543.396000
 Sum of electronic and thermal Free Energies=         -543.437165

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.593             31.408             86.640
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.844227	-0.945159	-0.000005
2	6	0	-2.707541	0.421434	-0.000072
3	6	0	-0.726072	-0.632970	-0.000067
4	6	0	-0.629485	1.833721	0.000220
5	6	0	1.285375	0.679692	0.000073
6	6	0	2.798360	-0.923935	0.000129
7	7	0	0.673231	1.889456	0.000197
8	7	0	-1.336259	0.652509	0.000079
9	7	0	-1.630281	-1.591232	-0.000167
10	7	0	2.642727	0.441236	-0.000110
11	7	0	1.655116	-1.576113	-0.000214
12	6	0	0.695311	-0.589553	-0.000062
13	1	0	3.776501	-1.386435	0.000165
14	1	0	3.368426	1.145214	-0.000120
15	1	0	-1.214675	2.747987	0.000254
16	1	0	-3.423160	1.229842	-0.000084
17	1	0	-3.769154	-1.506981	-0.000007

1,N^6-ethenoadenine: N9H N9 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.990051456     A.U.
 Zero-point correction=                           0.110312
(Hartree/Particle)
 Thermal correction to Energy=                    0.117700
 Thermal correction to Enthalpy=                  0.118645
 Thermal correction to Gibbs Free Energy=         0.077813
 Sum of electronic and zero-point Energies=           -542.879739
 Sum of electronic and thermal Energies=              -542.872351
```

```
 Sum of electronic and thermal Enthalpies=            -542.871407
 Sum of electronic and thermal Free Energies=         -542.912238

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.858             30.228             85.937

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0       -2.814776   -0.943070    0.000059
    2          6             0       -2.673253    0.426515    0.000031
    3          6             0       -0.685936   -0.627258   -0.000018
    4          6             0       -0.583041    1.832615    0.000081
    5          6             0        1.372269    0.687617    0.000019
    6          6             0        2.824345   -0.839895   -0.000123
    7          7             0        0.716548    1.889841    0.000063
    8          7             0       -1.298069    0.647107    0.000049
    9          7             0       -1.610026   -1.594753    0.000002
   10          7             0        2.722058    0.506230   -0.000155
   11          7             0        1.681983   -1.566834    0.000016
   12          6             0        0.731326   -0.590827   -0.000037
   13          1             0        3.795153   -1.329088   -0.000151
   14          1             0       -1.180334    2.741671    0.000108
   15          1             0       -3.382413    1.241696    0.000066
   16          1             0       -3.745474   -1.499600    0.000085
 -----------------------------------------------------------------------
```

1,N^6-ethenoadenine: N9H C8 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.922696652     A.U.
Zero-point correction=                           0.109193
(Hartree/Particle)
 Thermal correction to Energy=                    0.116881
 Thermal correction to Enthalpy=                  0.117825
 Thermal correction to Gibbs Free Energy=         0.076527
 Sum of electronic and zero-point Energies=           -542.813505
 Sum of electronic and thermal Energies=              -542.805817
 Sum of electronic and thermal Enthalpies=            -542.804873
 Sum of electronic and thermal Free Energies=         -542.846171

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.344             31.576             86.920

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0        2.820793   -0.911098    0.000122
```

2	6	0	2.663404	0.457857	0.000090
3	6	0	0.689026	-0.624809	0.000056
4	6	0	0.565325	1.838510	-0.000063
5	6	0	-1.345621	0.650315	-0.000095
6	6	0	-2.913866	-1.036056	-0.000070
7	7	0	-0.744832	1.863199	-0.000113
8	7	0	1.286976	0.664259	0.000012
9	7	0	1.627013	-1.576779	0.000104
10	7	0	-2.686506	0.359761	-0.000002
11	7	0	-1.671507	-1.616429	-0.000057
12	6	0	-0.731655	-0.623432	-0.000002
13	1	0	-3.424326	1.048604	-0.000011
14	1	0	1.139162	2.760547	-0.000068
15	1	0	3.364005	1.280333	0.000072
16	1	0	3.758718	-1.455278	0.000167

1,N^6-ethenoadenine: N9H C2 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.929510913 A.U.
Zero-point correction= 0.109358
(Hartree/Particle)
Thermal correction to Energy= 0.117047
Thermal correction to Enthalpy= 0.117992
Thermal correction to Gibbs Free Energy= 0.076662
Sum of electronic and zero-point Energies= -542.820154
Sum of electronic and thermal Energies= -542.812465
Sum of electronic and thermal Enthalpies= -542.811520
Sum of electronic and thermal Free Energies= -542.852850

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.448	31.498	86.986

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.869999	-0.880391	-0.000006
2	6	0	-2.684386	0.481016	-0.000009
3	6	0	-0.746658	-0.602646	-0.000065
4	6	0	-0.675441	1.976986	0.000245
5	6	0	1.251955	0.688979	0.000060
6	6	0	2.788109	-0.920410	-0.000039
7	7	0	0.666026	1.911895	0.000219
8	7	0	-1.314010	0.687415	0.000101
9	7	0	-1.668517	-1.561351	-0.000186
10	7	0	2.617176	0.446711	0.000033
11	7	0	1.646509	-1.576112	-0.000266
12	6	0	0.676943	-0.585215	-0.000088
13	1	0	3.326834	1.165328	0.000169
14	1	0	-3.360350	1.322731	0.000012

15	1	0	-3.810041	-1.420734	-0.000015
16	1	0	3.770141	-1.377141	-0.000052

1,N^6-ethenoadenine: N9H C11 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.892426139 A.U.
Zero-point correction= 0.108714
(Hartree/Particle)
Thermal correction to Energy= 0.116575
Thermal correction to Enthalpy= 0.117520
Thermal correction to Gibbs Free Energy= 0.075878
Sum of electronic and zero-point Energies= -542.783712
Sum of electronic and thermal Energies= -542.775851
Sum of electronic and thermal Enthalpies= -542.774907
Sum of electronic and thermal Free Energies= -542.816548

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.152	32.002	87.641

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.976216	-1.050189	-0.000011
2	6	0	-2.765358	0.324191	0.000039
3	6	0	-0.762280	-0.678789	-0.000018
4	6	0	-0.704958	1.791382	0.000093
5	6	0	1.234542	0.691686	0.000000
6	6	0	2.787873	-0.884652	0.000013
7	7	0	0.612152	1.896258	0.000066
8	7	0	-1.390132	0.621162	0.000048
9	7	0	-1.652280	-1.633695	-0.000082
10	7	0	2.603793	0.479353	0.000014
11	7	0	1.657896	-1.556482	-0.000173
12	6	0	0.664269	-0.588436	-0.000038
13	1	0	3.309729	1.200879	0.000163
14	1	0	-3.472331	1.147143	0.000080
15	1	0	3.776836	-1.326148	0.000030
16	1	0	-1.301470	2.700798	0.000147

1,N^6-ethenoadenine: N9H C12 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.922527985   A.U.
 Zero-point correction=   0.110029
(Hartree/Particle)
 Thermal correction to Energy=   0.117683
 Thermal correction to Enthalpy=   0.118627
 Thermal correction to Gibbs Free Energy=   0.077356
 Sum of electronic and zero-point Energies=   -542.812499
 Sum of electronic and thermal Energies=   -542.804845
 Sum of electronic and thermal Enthalpies=   -542.803901
 Sum of electronic and thermal Free Energies=   -542.845172

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.847	31.195	86.862

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.894413	-0.857515	-0.000130
2	6	0	-2.804649	0.533063	0.000018
3	6	0	-0.766543	-0.639554	-0.000045
4	6	0	-0.671881	1.816683	0.000085
5	6	0	1.248046	0.673550	0.000050
6	6	0	2.778592	-0.925141	-0.000003
7	7	0	0.643038	1.890922	0.000098
8	7	0	-1.392432	0.662120	0.000014
9	7	0	-1.685339	-1.570579	-0.000079
10	7	0	2.613533	0.440339	-0.000025
11	7	0	1.636578	-1.580116	0.000023
12	6	0	0.658415	-0.595281	-0.000016
13	1	0	3.329198	1.152250	0.000078
14	1	0	3.760861	-1.381156	-0.000022
15	1	0	-1.265882	2.725587	0.000131
16	1	0	-3.817228	-1.430322	-0.000170

1,N^6-ethenoadenine: N9H N7 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.896499872   A.U.
 Zero-point correction=   0.137793
(Hartree/Particle)
 Thermal correction to Energy=   0.145464
 Thermal correction to Enthalpy=   0.146408
 Thermal correction to Gibbs Free Energy=   0.105114
 Sum of electronic and zero-point Energies=   -543.758707
 Sum of electronic and thermal Energies=   -543.751036
 Sum of electronic and thermal Enthalpies=   -543.750092
 Sum of electronic and thermal Free Energies=   -543.791386

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.280	32.036	86.911

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.854646	-0.974448	0.000111
2	6	0	2.741980	0.396929	-0.000031
3	6	0	0.754789	-0.614940	0.000055
4	6	0	0.679850	1.848431	-0.000175
5	6	0	-1.249345	0.718018	-0.000081
6	6	0	-2.855124	-0.823315	0.000070
7	7	0	-0.624457	1.912478	-0.000182
8	7	0	1.380870	0.662374	-0.000066
9	7	0	1.623726	-1.593172	0.000146
10	7	0	-2.621377	0.494484	0.000022
11	7	0	-1.676634	-1.466186	0.000087
12	6	0	-0.654514	-0.536246	0.000033
13	1	0	-3.332743	1.220373	-0.000014
14	1	0	-3.827620	-1.293557	0.000115
15	1	0	1.265413	2.762354	-0.000252
16	1	0	3.766710	-1.555346	0.000176
17	1	0	3.480033	1.185280	-0.000111
18	1	0	-1.560367	-2.475526	0.000142

1,N^6-ethenoadenine: N9H N10 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.910604344 A.U.
Zero-point correction= 0.137756
(Hartree/Particle)
Thermal correction to Energy= 0.145447
Thermal correction to Enthalpy= 0.146392
Thermal correction to Gibbs Free Energy= 0.105097
Sum of electronic and zero-point Energies= -543.772848
Sum of electronic and thermal Energies= -543.765157
Sum of electronic and thermal Enthalpies= -543.764213
Sum of electronic and thermal Free Energies= -543.805507

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.270	32.202	86.911

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.893791	-0.859027	0.000056
2	6	0	2.689938	0.482170	-0.000006
3	6	0	0.680315	-0.551793	0.000020
4	6	0	0.575958	1.868413	-0.000045
5	6	0	-1.333207	0.693700	-0.000037
6	6	0	-2.798637	-0.953980	0.000088
7	7	0	-0.724515	1.896500	-0.000064

8	7	0	1.301121	0.683475	-0.000010
9	7	0	1.653793	-1.483874	0.000053
10	7	0	-2.673410	0.417320	-0.000040
11	7	0	-1.641096	-1.583411	-0.000014
12	6	0	-0.718234	-0.572108	0.000004
13	1	0	-3.424459	1.099283	-0.000128
14	1	0	-3.766409	-1.438143	0.000128
15	1	0	1.156304	2.784701	-0.000076
16	1	0	3.814324	-1.423222	0.000092
17	1	0	3.386362	1.306459	-0.000040
18	1	0	1.483084	-2.483383	0.000067

1,N^6-ethenoadenine: N9H N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.869075481 A.U.
Zero-point correction= 0.136555
(Hartree/Particle)
Thermal correction to Energy= 0.144491
Thermal correction to Enthalpy= 0.145435
Thermal correction to Gibbs Free Energy= 0.103705
Sum of electronic and zero-point Energies= -543.732521
Sum of electronic and thermal Energies= -543.724584
Sum of electronic and thermal Enthalpies= -543.723640
Sum of electronic and thermal Free Energies= -543.765370

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.670	33.042	87.828

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.844175	-0.980697	0.000023
2	6	0	-2.740222	0.385398	-0.000029
3	6	0	-0.725139	-0.662891	-0.000036
4	6	0	-0.716978	1.815571	0.000121
5	6	0	1.317789	0.639804	0.000024
6	6	0	2.789490	-0.980203	0.000119
7	7	0	0.622313	1.824277	0.000090
8	7	0	-1.371497	0.652557	0.000059
9	7	0	-1.613261	-1.607668	-0.000092
10	7	0	2.663657	0.398930	-0.000091
11	7	0	1.636161	-1.603178	-0.000164
12	6	0	0.693219	-0.610147	-0.000042
13	1	0	3.425333	1.067383	-0.000063
14	1	0	3.761767	-1.455264	0.000149
15	1	0	-1.252964	2.756682	0.000152
16	1	0	-3.756929	-1.561384	0.000018
17	1	0	-3.478668	1.173265	-0.000040
18	1	0	1.095953	2.723882	0.000094

1,N^6-ethenoadenine: N9H N1 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.795620888     A.U.
 Zero-point correction=                           0.134754
(Hartree/Particle)
 Thermal correction to Energy=                    0.142790
 Thermal correction to Enthalpy=                  0.143734
 Thermal correction to Gibbs Free Energy=         0.101684
 Sum of electronic and zero-point Energies=           -543.660867
 Sum of electronic and thermal Energies=              -543.652831
 Sum of electronic and thermal Enthalpies=            -543.651887
 Sum of electronic and thermal Free Energies=         -543.693937

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.602             33.240             88.502
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.810263	-0.973719	-0.245045
2	6	0	-2.768099	0.338304	0.045359
3	6	0	-0.675932	-0.721516	0.094318
4	6	0	-0.627492	1.881806	-0.097264
5	6	0	1.291089	0.674683	-0.016520
6	6	0	2.846854	-0.877733	-0.001661
7	7	0	0.634216	1.864082	-0.209412
8	7	0	-1.363916	0.645050	0.383265
9	7	0	-1.546863	-1.600538	-0.204461
10	7	0	2.639521	0.474968	-0.106949
11	7	0	1.722108	-1.557252	0.130306
12	6	0	0.746477	-0.605072	0.137544
13	1	0	3.343951	1.194551	-0.235438
14	1	0	3.837610	-1.311854	-0.017573
15	1	0	-1.251791	2.757175	-0.241142
16	1	0	-3.686021	-1.556078	-0.500701
17	1	0	-3.525214	1.104522	0.127343
18	1	0	-1.329793	0.726996	1.417877

1,N^6-ethenoadenine: N9H N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.822991661     A.U.
 Zero-point correction=                           0.136075
(Hartree/Particle)
 Thermal correction to Energy=                    0.143950
 Thermal correction to Enthalpy=                  0.144894
 Thermal correction to Gibbs Free Energy=         0.103188
 Sum of electronic and zero-point Energies=           -543.686917
 Sum of electronic and thermal Energies=              -543.679041
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```
 Sum of electronic and thermal Enthalpies=            -543.678097
 Sum of electronic and thermal Free Energies=         -543.719804

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.330             32.542             87.779

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.866814   -0.966270   -0.000072
    2          6             0       -2.746912    0.408635   -0.000084
    3          6             0       -0.761966   -0.634125   -0.000069
    4          6             0       -0.690326    1.841170    0.000153
    5          6             0        1.209677    0.686757    0.000088
    6          6             0        2.762438   -1.044939   -0.000035
    7          7             0        0.624697    1.882345    0.000182
    8          7             0       -1.391497    0.665626    0.000028
    9          7             0       -1.647830   -1.595528   -0.000178
   10          7             0        2.678615    0.484810    0.000091
   11          7             0        1.620182   -1.588112   -0.000108
   12          6             0        0.647746   -0.567197   -0.000033
   13          1             0        3.136258    0.895949    0.828881
   14          1             0        3.743275   -1.505529   -0.000058
   15          1             0       -1.259389    2.764927    0.000192
   16          1             0       -3.785110   -1.538187   -0.000105
   17          1             0       -3.483551    1.198571   -0.000084
   18          1             0        3.136284    0.896089   -0.828617
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: NEUTRAL N7H
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.529729806     A.U.
 Zero-point correction=                           0.124132
(Hartree/Particle)
 Thermal correction to Energy=                    0.131725
 Thermal correction to Enthalpy=                  0.132670
 Thermal correction to Gibbs Free Energy=         0.091502
 Sum of electronic and zero-point Energies=           -543.405598
 Sum of electronic and thermal Energies=              -543.398004
 Sum of electronic and thermal Enthalpies=            -543.397060
 Sum of electronic and thermal Free Energies=         -543.438228

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.659             31.341             86.645

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.819375   -0.977243    0.000032
```

2	6	0	-2.708802	0.393594	0.000097
3	6	0	-0.715184	-0.606487	-0.000016
4	6	0	-0.637156	1.846302	0.000144
5	6	0	1.327384	0.723658	0.000016
6	6	0	2.881232	-0.736388	-0.000154
7	7	0	0.658403	1.915930	0.000102
8	7	0	-1.344170	0.654276	0.000091
9	7	0	-1.591130	-1.597023	-0.000034
10	7	0	2.695638	0.563653	-0.000158
11	7	0	1.703022	-1.451655	-0.000082
12	6	0	0.692003	-0.524671	-0.000047
13	1	0	1.595054	-2.456983	-0.000067
14	1	0	3.843159	-1.231708	-0.000211
15	1	0	-3.732188	-1.558136	0.000025
16	1	0	-3.441615	1.186362	0.000171
17	1	0	-1.237363	2.751595	0.000212

1,N^6-ethenoadenine: N7H N7 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.990051456     A.U.
 Zero-point correction=                           0.110312
(Hartree/Particle)
 Thermal correction to Energy=                    0.117700
 Thermal correction to Enthalpy=                  0.118645
 Thermal correction to Gibbs Free Energy=         0.077813
 Sum of electronic and zero-point Energies=           -542.879739
 Sum of electronic and thermal Energies=              -542.872351
 Sum of electronic and thermal Enthalpies=            -542.871407
 Sum of electronic and thermal Free Energies=         -542.912238

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.858             30.228             85.937
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.814776	-0.943070	0.000059
2	6	0	-2.673253	0.426515	0.000031
3	6	0	-0.685936	-0.627258	-0.000018
4	6	0	-0.583041	1.832615	0.000081
5	6	0	1.372269	0.687617	0.000019
6	6	0	2.824345	-0.839895	-0.000123
7	7	0	0.716548	1.889841	0.000063
8	7	0	-1.298069	0.647107	0.000049
9	7	0	-1.610026	-1.594753	0.000002
10	7	0	2.722058	0.506230	-0.000155
11	7	0	1.681983	-1.566834	0.000016
12	6	0	0.731326	-0.590827	-0.000037
13	1	0	3.795153	-1.329088	-0.000151
14	1	0	-3.745474	-1.499600	0.000085
15	1	0	-3.382413	1.241696	0.000066

16	1	0	-1.180334	2.741671	0.000108

1,N^6-ethenoadenine: N7H C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.925401180 A.U.

Zero-point correction= 0.109313
(Hartree/Particle)
Thermal correction to Energy= 0.117006
Thermal correction to Enthalpy= 0.117950
Thermal correction to Gibbs Free Energy= 0.076628
Sum of electronic and zero-point Energies= -542.816088
Sum of electronic and thermal Energies= -542.808395
Sum of electronic and thermal Enthalpies= -542.807451
Sum of electronic and thermal Free Energies= -542.848773

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.422	31.542	86.969

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.804295	-0.934441	0.000107
2	6	0	-2.671376	0.436658	-0.000034
3	6	0	-0.680945	-0.601626	-0.000053
4	6	0	-0.566447	1.841657	0.000199
5	6	0	1.397415	0.682559	0.000085
6	6	0	3.004844	-0.846288	0.000002
7	7	0	0.735376	1.884281	0.000184
8	7	0	-1.295439	0.668273	0.000091
9	7	0	-1.597345	-1.582491	-0.000072
10	7	0	2.748982	0.492911	-0.000296
11	7	0	1.732345	-1.481718	-0.000128
12	6	0	0.720115	-0.561235	-0.000080
13	1	0	-3.733363	-1.493329	0.000165
14	1	0	-3.387494	1.245256	-0.000064
15	1	0	-1.151249	2.758763	0.000222
16	1	0	1.608794	-2.483178	-0.000131

1,N^6-ethenoadenine: N7H C2 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.924483305 A.U.
Zero-point correction= 0.109077
(Hartree/Particle)
Thermal correction to Energy= 0.116888
Thermal correction to Enthalpy= 0.117832
Thermal correction to Gibbs Free Energy= 0.076263

```
 Sum of electronic and zero-point Energies=          -542.815406
 Sum of electronic and thermal Energies=             -542.807596
 Sum of electronic and thermal Enthalpies=           -542.806651
 Sum of electronic and thermal Free Energies=        -542.848220

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.348             31.785             87.489

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.841911   -0.918067    0.000105
    2          6             0        2.686522    0.450697   -0.000203
    3          6             0        0.735471   -0.571218   -0.000025
    4          6             0        0.681061    2.002144    0.000014
    5          6             0       -1.298992    0.739792    0.000088
    6          6             0       -2.860972   -0.745107    0.000365
    7          7             0       -0.651766    1.945706    0.000004
    8          7             0        1.325387    0.691691    0.000009
    9          7             0        1.623612   -1.569088   -0.000014
   10          7             0       -2.681750    0.557850   -0.000457
   11          7             0       -1.679782   -1.452849    0.000073
   12          6             0       -0.672370   -0.508976    0.000010
   13          1             0        3.769556   -1.479358    0.000193
   14          1             0        3.386108    1.273280   -0.000355
   15          1             0       -1.560480   -2.455264    0.000135
   16          1             0       -3.820872   -1.247428    0.000601
```

1,N^6-ethenoadenine: N7H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.900707699     A.U.
  Zero-point correction=                           0.109220
(Hartree/Particle)
 Thermal correction to Energy=                     0.116972
 Thermal correction to Enthalpy=                   0.117916
 Thermal correction to Gibbs Free Energy=          0.076461
 Sum of electronic and zero-point Energies=           -542.791488
 Sum of electronic and thermal Energies=              -542.783736
 Sum of electronic and thermal Enthalpies=            -542.782792
 Sum of electronic and thermal Free Energies=         -542.824247

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.401             31.642             87.249

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.937320   -1.095261    0.000020
    2          6             0        2.763744    0.289303   -0.000143
```

3	6	0	0.748771	-0.639593	-0.000020
4	6	0	0.708496	1.807541	-0.000004
5	6	0	-1.282800	0.743116	0.000021
6	6	0	-2.857174	-0.709131	0.000264
7	7	0	-0.598057	1.928104	-0.000012
8	7	0	1.397458	0.623185	-0.000023
9	7	0	1.601670	-1.638346	0.000003
10	7	0	-2.660735	0.591846	-0.000195
11	7	0	-1.681924	-1.430106	0.000071
12	6	0	-0.657671	-0.510777	0.000007
13	1	0	3.495369	1.089790	-0.000233
14	1	0	-1.566009	-2.433424	0.000116
15	1	0	-3.823612	-1.196936	0.000434
16	1	0	1.321255	2.706602	-0.000085

1,N^6-ethenoadenine: N7H C12 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.927965518 A.U.
Zero-point correction= 0.110240
(Hartree/Particle)
Thermal correction to Energy= 0.117844
Thermal correction to Enthalpy= 0.118788
Thermal correction to Gibbs Free Energy= 0.077599
Sum of electronic and zero-point Energies= -542.817725
Sum of electronic and thermal Energies= -542.810122
Sum of electronic and thermal Enthalpies= -542.809178
Sum of electronic and thermal Free Energies= -542.850366

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.948	31.028	86.689

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.865057	-0.896270	0.000071
2	6	0	-2.805127	0.501126	0.000043
3	6	0	-0.754146	-0.604888	-0.000031
4	6	0	-0.675927	1.832646	0.000177
5	6	0	1.296633	0.722952	0.000027
6	6	0	2.853075	-0.749836	-0.000070
7	7	0	0.629547	1.922151	0.000130
8	7	0	-1.400493	0.664924	0.000094
9	7	0	-1.639895	-1.577130	-0.000049
10	7	0	2.671449	0.552980	-0.000231
11	7	0	1.666539	-1.455369	-0.000099
12	6	0	0.652914	-0.520430	-0.000060
13	1	0	1.542005	-2.457243	-0.000087
14	1	0	3.812739	-1.251144	-0.000061
15	1	0	-1.284012	2.733111	0.000219

16	1	0	-3.774941	-1.489419	0.000079

1,N^6-ethenoadenine: N7H N9 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.896499872 A.U.
ZZero-point correction= 0.137793
(Hartree/Particle)
Thermal correction to Energy= 0.145464
Thermal correction to Enthalpy= 0.146408
Thermal correction to Gibbs Free Energy= 0.105114
Sum of electronic and zero-point Energies= -543.758707
Sum of electronic and thermal Energies= -543.751036
Sum of electronic and thermal Enthalpies= -543.750092
Sum of electronic and thermal Free Energies= -543.791386

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.280	32.036	86.911

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.854646	-0.974448	0.000111
2	6	0	2.741980	0.396929	-0.000031
3	6	0	0.754789	-0.614940	0.000055
4	6	0	0.679850	1.848431	-0.000175
5	6	0	-1.249345	0.718018	-0.000081
6	6	0	-2.855124	-0.823315	0.000070
7	7	0	-0.624457	1.912478	-0.000182
8	7	0	1.380870	0.662374	-0.000066
9	7	0	1.623726	-1.593172	0.000146
10	7	0	-2.621377	0.494484	0.000022
11	7	0	-1.676634	-1.466186	0.000087
12	6	0	-0.654514	-0.536246	0.000033
13	1	0	-1.560367	-2.475526	0.000142
14	1	0	-3.827620	-1.293557	0.000115
15	1	0	1.265413	2.762354	-0.000252
16	1	0	3.766710	-1.555346	0.000176
17	1	0	3.480033	1.185280	-0.000111
18	1	0	-3.332743	1.220373	-0.000014

1,N^6-ethenoadenine: N7H N10 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.894986097 A.U.
Zero-point correction= 0.137070
(Hartree/Particle)
Thermal correction to Energy= 0.144942

```
 Thermal correction to Enthalpy=                  0.145887
 Thermal correction to Gibbs Free Energy=         0.104264
 Sum of electronic and zero-point Energies=           -543.757918
 Sum of electronic and thermal Energies=              -543.750045
 Sum of electronic and thermal Enthalpies=            -543.749101
 Sum of electronic and thermal Free Energies=         -543.790723

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.953             32.785            87.603

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.895786   -0.866172    0.000096
    2          6             0       -2.689865    0.472930    0.000079
    3          6             0       -0.673921   -0.554877   -0.000012
    4          6             0       -0.585514    1.868082    0.000146
    5          6             0        1.365221    0.723078    0.000034
    6          6             0        2.909219   -0.736338   -0.000125
    7          7             0        0.707399    1.910077    0.000103
    8          7             0       -1.303467    0.675080    0.000094
    9          7             0       -1.654093   -1.492350   -0.000013
   10          7             0        2.719724    0.562681   -0.000268
   11          7             0        1.737506   -1.462766   -0.000084
   12          6             0        0.719569   -0.539406   -0.000048
   13          1             0        1.673233   -2.473315   -0.000057
   14          1             0        3.874165   -1.227215   -0.000176
   15          1             0       -1.181478    2.775303    0.000190
   16          1             0       -3.814945   -1.432585    0.000124
   17          1             0       -3.384541    1.298929    0.000118
   18          1             0       -1.509463   -2.493958   -0.000039
 ---------------------------------------------------------------------
```

1,N^6-ethenoadenine: N7H N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.888415227     A.U.
Zero-point correction=                           0.137488
(Hartree/Particle)
 Thermal correction to Energy=                    0.145219
 Thermal correction to Enthalpy=                  0.146163
 Thermal correction to Gibbs Free Energy=         0.104785
 Sum of electronic and zero-point Energies=           -543.750927
 Sum of electronic and thermal Energies=              -543.743196
 Sum of electronic and thermal Enthalpies=            -543.742252
 Sum of electronic and thermal Free Energies=         -543.783631

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.126             32.296            87.088
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.830468	-0.994989	0.000095
2	6	0	-2.735088	0.372415	0.000084
3	6	0	-0.718943	-0.647041	-0.000037
4	6	0	-0.713054	1.822666	0.000183
5	6	0	1.342714	0.660262	-0.000040
6	6	0	2.883957	-0.770767	-0.000105
7	7	0	0.617392	1.832971	0.000099
8	7	0	-1.367909	0.651108	0.000120
9	7	0	-1.593756	-1.610595	-0.000003
10	7	0	2.690815	0.536353	-0.000303
11	7	0	1.709653	-1.484600	-0.000069
12	6	0	0.688136	-0.572061	-0.000084
13	1	0	1.612222	-2.494338	0.000007
14	1	0	3.851098	-1.255376	-0.000098
15	1	0	-1.260341	2.757370	0.000245
16	1	0	-3.738695	-1.582441	0.000129
17	1	0	-3.479486	1.154703	0.000136
18	1	0	1.118318	2.720509	0.000081

1,N^6-ethenoadenine: N7H N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.794249387 A.U.
Zero-point correction= 0.134816
(Hartree/Particle)
Thermal correction to Energy= 0.142864
Thermal correction to Enthalpy= 0.143808
Thermal correction to Gibbs Free Energy= 0.101706
Sum of electronic and zero-point Energies= -543.659433
Sum of electronic and thermal Energies= -543.651385
Sum of electronic and thermal Enthalpies= -543.650441
Sum of electronic and thermal Free Energies= -543.692543

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.649	33.224	88.612

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.781729	-1.010997	-0.254907
2	6	0	-2.771182	0.305384	0.023181
3	6	0	-0.666842	-0.689117	0.114426
4	6	0	-0.629945	1.900447	-0.096809
5	6	0	1.334296	0.716920	-0.018847
6	6	0	2.918723	-0.693043	-0.039252
7	7	0	0.622975	1.895232	-0.200670
8	7	0	-1.377791	0.641246	0.382089
9	7	0	-1.505705	-1.607511	-0.190818

10	7	0	2.676965	0.604801	-0.135686
11	7	0	1.777794	-1.433200	0.114882
12	6	0	0.737991	-0.541349	0.160296
13	1	0	1.717142	-2.442622	0.200326
14	1	0	3.899371	-1.149030	-0.070419
15	1	0	-1.274937	2.763397	-0.228411
16	1	0	-3.640688	-1.613589	-0.520335
17	1	0	-3.543142	1.058204	0.087906
18	1	0	-1.365289	0.750197	1.413828

1,N^6-ethenoadenine: N7H N7 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.822996284 A.U.
Zero-point correction= 0.136110
(Hartree/Particle)
Thermal correction to Energy= 0.144002
Thermal correction to Enthalpy= 0.144946
Thermal correction to Gibbs Free Energy= 0.103173
Sum of electronic and zero-point Energies= -543.686887
Sum of electronic and thermal Energies= -543.678995
Sum of electronic and thermal Enthalpies= -543.678051
Sum of electronic and thermal Free Energies= -543.719823

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.362	32.542	87.917

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.823424	-1.011135	-0.000048
2	6	0	2.745147	0.367862	-0.000122
3	6	0	0.736189	-0.597686	0.000011
4	6	0	0.705910	1.858223	-0.000136
5	6	0	-1.261868	0.763282	-0.000003
6	6	0	-2.970294	-0.586381	0.000139
7	7	0	-0.599176	1.935016	-0.000097
8	7	0	1.396678	0.666764	-0.000089
9	7	0	1.582966	-1.601268	0.000044
10	7	0	-2.673776	0.638293	0.000061
11	7	0	-1.704081	-1.486698	0.000153
12	6	0	-0.655668	-0.473093	0.000054
13	1	0	-1.674967	-2.101815	0.828810
14	1	0	-3.935980	-1.077166	0.000202
15	1	0	1.301493	2.766137	-0.000214
16	1	0	3.723457	-1.611132	-0.000049
17	1	0	3.505697	1.134721	-0.000195
18	1	0	-1.675021	-2.101918	-0.828430

1,N^6-ethenoadenine: NEUTRAL C5H
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.475952681     A.U.
 Zero-point correction=                           0.122787
(Hartree/Particle)
 Thermal correction to Energy=                    0.130505
 Thermal correction to Enthalpy=                  0.131449
 Thermal correction to Gibbs Free Energy=         0.089695
 Sum of electronic and zero-point Energies=           -543.353166
 Sum of electronic and thermal Energies=              -543.345448
 Sum of electronic and thermal Enthalpies=            -543.344504
 Sum of electronic and thermal Free Energies=         -543.386257

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  81.893             30.940             87.877

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.748372   -0.973298   -0.231827
    2          6             0       -2.628527    0.386913   -0.252796
    3          6             0       -0.672399   -0.609878    0.169525
    4          6             0       -0.593114    1.846904    0.081340
    5          6             0        1.366664    0.740720    0.112725
    6          6             0        2.671632   -0.867045   -0.375369
    7          7             0        0.689081    1.948438    0.137611
    8          7             0       -1.279153    0.637291    0.003220
    9          7             0       -1.528917   -1.583545    0.046500
   10          7             0        2.524340    0.543827   -0.432984
   11          7             0        1.717885   -1.571504    0.136273
   12          6             0        0.763657   -0.567401    0.596527
   13          1             0        0.786162   -0.607549    1.700572
   14          1             0        3.577919   -1.314132   -0.772163
   15          1             0       -1.214673    2.739388    0.074087
   16          1             0       -3.333049    1.185034   -0.434544
   17          1             0       -3.636249   -1.565786   -0.403040
 ---------------------------------------------------------------------
```

1,N^6-ethenoadenine: C5H C8 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.857849274     A.U.
 Zero-point correction=                           0.106778
(Hartree/Particle)
 Thermal correction to Energy=                    0.114754
 Thermal correction to Enthalpy=                  0.115699
 Thermal correction to Gibbs Free Energy=         0.073583
 Sum of electronic and zero-point Energies=           -542.751071
 Sum of electronic and thermal Energies=              -542.743095
```

```
 Sum of electronic and thermal Enthalpies=            -542.742151
 Sum of electronic and thermal Free Energies=         -542.784267

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.009             32.016             88.641

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0       -2.729699   -0.927394   -0.210997
    2          6             0       -2.561956    0.429355   -0.322347
    3          6             0       -0.643391   -0.600579    0.210041
    4          6             0       -0.516829    1.851501    0.094043
    5          6             0        1.423594    0.687625    0.147739
    6          6             0        2.757780   -0.980895   -0.488756
    7          7             0        0.760729    1.914455    0.245229
    8          7             0       -1.213108    0.647776   -0.056121
    9          7             0       -1.549205   -1.558700    0.128410
   10          7             0        2.520095    0.507603   -0.503821
   11          7             0        1.766718   -1.626616    0.047678
   12          6             0        0.793185   -0.613889    0.595652
   13          1             0        0.868271   -0.757489    1.685555
   14          1             0       -1.130810    2.750295    0.083046
   15          1             0       -3.231427    1.236391   -0.583568
   16          1             0       -3.638744   -1.495165   -0.366913
 -----------------------------------------------------------------------
```

1,N^6-ethenoadenine: C5H C5 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.990051456     A.U.
 Zero-point correction=                           0.110312
(Hartree/Particle)
 Thermal correction to Energy=                    0.117700
 Thermal correction to Enthalpy=                  0.118645
 Thermal correction to Gibbs Free Energy=         0.077813
 Sum of electronic and zero-point Energies=           -542.879739
 Sum of electronic and thermal Energies=              -542.872351
 Sum of electronic and thermal Enthalpies=            -542.871407
 Sum of electronic and thermal Free Energies=         -542.912238

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.858             30.228             85.937

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0       -2.814776   -0.943070    0.000059
    2          6             0       -2.673253    0.426515    0.000031
    3          6             0       -0.685936   -0.627258   -0.000018
```

4	6	0	-0.583041	1.832615	0.000081
5	6	0	1.372269	0.687617	0.000019
6	6	0	2.824345	-0.839895	-0.000123
7	7	0	0.716548	1.889841	0.000063
8	7	0	-1.298069	0.647107	0.000049
9	7	0	-1.610026	-1.594753	0.000002
10	7	0	2.722058	0.506230	-0.000155
11	7	0	1.681983	-1.566834	0.000016
12	6	0	0.731326	-0.590827	-0.000037
13	1	0	-1.180334	2.741671	0.000108
14	1	0	-3.382413	1.241696	0.000066
15	1	0	-3.745474	-1.499600	0.000085
16	1	0	3.795153	-1.329088	-0.000151

1,N^6-ethenoadenine: C5H C2 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.897241114     A.U.
 Zero-point correction=                           0.108276
(Hartree/Particle)
 Thermal correction to Energy=                    0.116076
 Thermal correction to Enthalpy=                  0.117020
 Thermal correction to Gibbs Free Energy=         0.075115
 Sum of electronic and zero-point Energies=           -542.788965
 Sum of electronic and thermal Energies=              -542.781165
 Sum of electronic and thermal Enthalpies=            -542.780221
 Sum of electronic and thermal Free Energies=         -542.822126
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.839	30.926	88.197

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.767637	-0.912730	-0.230265
2	6	0	-2.597848	0.450429	-0.264483
3	6	0	-0.692530	-0.568840	0.157335
4	6	0	-0.634546	2.010178	0.131626
5	6	0	1.338220	0.758195	0.096873
6	6	0	2.640466	-0.866906	-0.370757
7	7	0	0.692417	1.952807	0.145835
8	7	0	-1.258659	0.676090	-0.022291
9	7	0	-1.568279	-1.549777	0.055423
10	7	0	2.515713	0.525509	-0.449289
11	7	0	1.689664	-1.576537	0.153994
12	6	0	0.739419	-0.551867	0.597765
13	1	0	-3.270391	1.278132	-0.435697
14	1	0	-3.673451	-1.483154	-0.395799
15	1	0	3.542988	-1.332295	-0.764802
16	1	0	0.751601	-0.570090	1.702043

1,N^6-ethenoadenine: C5H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.858840656     A.U.
  Zero-point correction=                           0.107662
(Hartree/Particle)
 Thermal correction to Energy=                    0.115542
 Thermal correction to Enthalpy=                  0.116486
 Thermal correction to Gibbs Free Energy=         0.074438
 Sum of electronic and zero-point Energies=           -542.751179
 Sum of electronic and thermal Energies=              -542.743299
 Sum of electronic and thermal Enthalpies=            -542.742355
 Sum of electronic and thermal Free Energies=         -542.784403

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.504             31.292             88.498

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.873450   -1.084765   -0.314325
    2          6             0       -2.723677    0.274423   -0.196594
    3          6             0       -0.710029   -0.658177    0.132122
    4          6             0       -0.692965    1.780249    0.095700
    5          6             0        1.314079    0.768352    0.068162
    6          6             0        2.695794   -0.803724   -0.313724
    7          7             0        0.613886    1.942313    0.064111
    8          7             0       -1.353987    0.600249    0.074709
    9          7             0       -1.534967   -1.638670   -0.022388
   10          7             0        2.521848    0.587770   -0.411299
   11          7             0        1.740679   -1.537595    0.164592
   12          6             0        0.734020   -0.553076    0.553096
   13          1             0       -3.425301    1.088172   -0.339054
   14          1             0        3.634147   -1.236435   -0.654526
   15          1             0        0.737605   -0.539952    1.660285
   16          1             0       -1.321297    2.670049    0.098605
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: C5H C12 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.888871656     A.U.
 Zero-point correction=                           0.109089
(Hartree/Particle)
 Thermal correction to Energy=                    0.116727
 Thermal correction to Enthalpy=                  0.117671
 Thermal correction to Gibbs Free Energy=         0.076075
 Sum of electronic and zero-point Energies=           -542.779783
 Sum of electronic and thermal Energies=              -542.772145
 Sum of electronic and thermal Enthalpies=            -542.771201
 Sum of electronic and thermal Free Energies=         -542.812796
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.247	30.357	87.546

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.822255	-0.878977	-0.213204
2	6	0	-2.756240	0.504848	-0.215179
3	6	0	-0.715523	-0.615466	0.103655
4	6	0	-0.642771	1.812161	0.062017
5	6	0	1.335542	0.740071	0.094530
6	6	0	2.681701	-0.856605	-0.316178
7	7	0	0.664427	1.934103	0.101712
8	7	0	-1.337145	0.649004	-0.000770
9	7	0	-1.596653	-1.561501	-0.001793
10	7	0	2.543025	0.543439	-0.372989
11	7	0	1.704238	-1.578962	0.128983
12	6	0	0.717530	-0.577329	0.542497
13	1	0	3.612851	-1.300900	-0.662504
14	1	0	0.730092	-0.599366	1.650467
15	1	0	-1.263139	2.704953	0.040969
16	1	0	-3.712951	-1.479482	-0.363757

1,N^6-ethenoadenine: C5H N7 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.836425108 A.U.
Zero-point correction= 0.135687
(Hartree/Particle)
Thermal correction to Energy= 0.143628
Thermal correction to Enthalpy= 0.144573
Thermal correction to Gibbs Free Energy= 0.102468
Sum of electronic and zero-point Energies= -543.700739
Sum of electronic and thermal Energies= -543.692797
Sum of electronic and thermal Enthalpies= -543.691853
Sum of electronic and thermal Free Energies= -543.733957

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.128	32.126	88.616

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.755724	-1.003208	-0.244567
2	6	0	-2.674671	0.356443	-0.262574
3	6	0	-0.693417	-0.587305	0.163864
4	6	0	-0.659030	1.848337	0.093285
5	6	0	1.326112	0.783010	0.129902

6	6	0	2.713901	-0.736068	-0.408493
7	7	0	0.641459	1.940762	0.128902
8	7	0	-1.326640	0.652002	0.000690
9	7	0	-1.511866	-1.579948	0.043524
10	7	0	2.514518	0.600858	-0.427185
11	7	0	1.722057	-1.449604	0.105849
12	6	0	0.729824	-0.524488	0.631850
13	1	0	3.616211	-1.196535	-0.798688
14	1	0	0.756291	-0.577541	1.734255
15	1	0	-1.263306	2.752171	0.101464
16	1	0	-3.621867	-1.623791	-0.424333
17	1	0	-3.403471	1.132649	-0.444867
18	1	0	1.717466	-2.455776	0.250114

1,N^6-ethenoadenine: C5H N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.832215624     A.U.
 Zero-point correction=                           0.135334
(Hartree/Particle)
 Thermal correction to Energy=                    0.143239
 Thermal correction to Enthalpy=                  0.144184
 Thermal correction to Gibbs Free Energy=         0.102203
 Sum of electronic and zero-point Energies=           -543.696882
 Sum of electronic and thermal Energies=              -543.688976
 Sum of electronic and thermal Enthalpies=            -543.688032
 Sum of electronic and thermal Free Energies=         -543.730013

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.884             32.227             88.356
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.816526	-0.955203	-0.212283
2	6	0	-2.703868	0.398027	-0.200546
3	6	0	-0.720112	-0.625941	0.119429
4	6	0	-0.654473	1.824842	0.069786
5	6	0	1.296636	0.742286	0.130944
6	6	0	2.708419	-0.930964	-0.302832
7	7	0	0.663692	1.914222	0.093494
8	7	0	-1.334193	0.654767	0.015565
9	7	0	-1.575162	-1.578149	0.006297
10	7	0	2.528789	0.489389	-0.288597
11	7	0	1.689892	-1.588474	0.096617
12	6	0	0.720596	-0.591017	0.533732
13	1	0	3.648163	-1.352086	-0.642806
14	1	0	0.733322	-0.638300	1.642320
15	1	0	-1.238499	2.741703	0.048491
16	1	0	-3.704919	-1.549918	-0.370651
17	1	0	-3.418068	1.197185	-0.334413
18	1	0	3.184828	1.186947	-0.635956

1,N^6-ethenoadenine: C5H N10 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.832460089     A.U.
 Zero-point correction=                           0.136000
(Hartree/Particle)
 Thermal correction to Energy=                    0.143866
 Thermal correction to Enthalpy=                  0.144810
 Thermal correction to Gibbs Free Energy=         0.102839
 Sum of electronic and zero-point Energies=           -543.696460
 Sum of electronic and thermal Energies=              -543.688595
 Sum of electronic and thermal Enthalpies=            -543.687650
 Sum of electronic and thermal Free Energies=         -543.729621

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.277             31.971             88.335
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.759923	-0.912907	-0.281218
2	6	0	-2.589693	0.436762	-0.282505
3	6	0	-0.628683	-0.514036	0.235002
4	6	0	-0.527661	1.915160	0.095572
5	6	0	1.410407	0.749151	0.106101
6	6	0	2.627114	-0.923291	-0.414156
7	7	0	0.743751	1.966047	0.120206
8	7	0	-1.251422	0.671086	0.037542
9	7	0	-1.529626	-1.476125	0.047121
10	7	0	2.520351	0.495978	-0.494497
11	7	0	1.673892	-1.577590	0.166854
12	6	0	0.795276	-0.526379	0.659368
13	1	0	3.492185	-1.410906	-0.851134
14	1	0	0.832555	-0.549829	1.763730
15	1	0	-1.150081	2.805529	0.097449
16	1	0	-3.630382	-1.517199	-0.487944
17	1	0	-3.282608	1.239279	-0.487827
18	1	0	-1.321320	-2.469405	0.116162

1,N^6-ethenoadenine: C5H N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.814045505     A.U.
 Zero-point correction=                           0.135416
(Hartree/Particle)
 Thermal correction to Energy=                    0.143331
 Thermal correction to Enthalpy=                  0.144275
 Thermal correction to Gibbs Free Energy=         0.102325
```

```
 Sum of electronic and zero-point Energies=           -543.678630
 Sum of electronic and thermal Energies=              -543.670715
 Sum of electronic and thermal Enthalpies=            -543.669771
 Sum of electronic and thermal Free Energies=         -543.711721

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.941             32.372             88.292

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.784343   -0.985680   -0.214467
    2          6             0       -2.691286    0.364920   -0.186949
    3          6             0       -0.680439   -0.658197    0.138677
    4          6             0       -0.681480    1.807491    0.035640
    5          6             0        1.386683    0.677702    0.110892
    6          6             0        2.723743   -0.900654   -0.330484
    7          7             0        0.643380    1.866667    0.114121
    8          7             0       -1.317870    0.637190    0.034249
    9          7             0       -1.535420   -1.600481    0.003480
   10          7             0        2.564369    0.528901   -0.362916
   11          7             0        1.728687   -1.601630    0.093672
   12          6             0        0.758205   -0.617737    0.546819
   13          1             0        3.654841   -1.329998   -0.682944
   14          1             0        0.784583   -0.669360    1.653431
   15          1             0       -1.248157    2.729564   -0.052343
   16          1             0       -3.666867   -1.588263   -0.377430
   17          1             0       -3.414661    1.156868   -0.315105
   18          1             0        1.121752    2.759594   -0.004615
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: C5H N1 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.741113938     A.U.
 Zero-point correction=                           0.133465
(Hartree/Particle)
 Thermal correction to Energy=                    0.141584
 Thermal correction to Enthalpy=                  0.142528
 Thermal correction to Gibbs Free Energy=         0.100123
 Sum of electronic and zero-point Energies=           -543.607649
 Sum of electronic and thermal Energies=              -543.599531
 Sum of electronic and thermal Enthalpies=            -543.598587
 Sum of electronic and thermal Free Energies=         -543.640992

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  88.845             33.054             89.248

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

1	6	0	-2.406555	-1.175639	-0.602327
2	6	0	-2.667987	0.064849	-0.162800
3	6	0	-0.527374	-0.688416	0.378183
4	6	0	-0.800417	1.842482	0.013945
5	6	0	1.257009	0.828104	-0.060181
6	6	0	2.691350	-0.730253	-0.327012
7	7	0	0.425304	1.927208	-0.230095
8	7	0	-1.454805	0.529133	0.539061
9	7	0	-1.095119	-1.608954	-0.278734
10	7	0	2.348591	0.610632	-0.694311
11	7	0	1.890362	-1.362798	0.461768
12	6	0	0.866998	-0.395354	0.790952
13	1	0	3.598782	-1.167557	-0.728578
14	1	0	0.920192	-0.165494	1.867857
15	1	0	-1.520970	2.647385	-0.097240
16	1	0	-3.068377	-1.834870	-1.148890
17	1	0	-3.545306	0.695000	-0.200853
18	1	0	-1.662797	0.684353	1.539313

1,N^6-ethenoadenine: NEUTRAL C8H
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.491242766 A.U.
Zero-point correction= 0.122764
(Hartree/Particle)
Thermal correction to Energy= 0.130446
Thermal correction to Enthalpy= 0.131391
Thermal correction to Gibbs Free Energy= 0.089890
Sum of electronic and zero-point Energies= -543.368479
Sum of electronic and thermal Energies= -543.360796
Sum of electronic and thermal Enthalpies= -543.359852
Sum of electronic and thermal Free Energies= -543.401353

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	81.856	31.110	87.346

1	6	0	2.857533	-0.946809	0.000201
2	6	0	2.702608	0.417854	-0.000486
3	6	0	0.737018	-0.637283	-0.000070
4	6	0	0.619068	1.833211	0.000141
5	6	0	-1.361204	0.726765	0.000079
6	6	0	-2.859334	-0.835972	0.000047
7	7	0	-0.661386	1.932378	0.000157
8	7	0	1.333017	0.630540	-0.000009
9	7	0	1.639300	-1.591860	-0.000021
10	7	0	-2.646112	0.602203	0.000063
11	7	0	-1.587775	-1.556228	-0.000022
12	6	0	-0.708057	-0.611771	-0.000055
13	1	0	-3.447260	-1.126019	0.882486
14	1	0	-3.447316	-1.125980	-0.882367
15	1	0	3.782950	-1.506278	0.000397

16	1	0	3.409880	1.234242	-0.000803
17	1	0	1.236649	2.728840	-0.000031

1,N^6-ethenoadenine: C8H C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.990052421 A.U.
Zero-point correction= 0.110305
(Hartree/Particle)
Thermal correction to Energy= 0.117692
Thermal correction to Enthalpy= 0.118636
Thermal correction to Gibbs Free Energy= 0.077808
Sum of electronic and zero-point Energies= -542.879748
Sum of electronic and thermal Energies= -542.872360
Sum of electronic and thermal Enthalpies= -542.871416
Sum of electronic and thermal Free Energies= -542.912245

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.853	30.228	85.932

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.814508	-0.943230	0.000530
2	6	0	2.673077	0.426439	-0.000224
3	6	0	0.686143	-0.626715	-0.000312
4	6	0	0.582942	1.833166	0.000009
5	6	0	-1.372042	0.687683	0.000230
6	6	0	-2.823940	-0.840079	-0.000146
7	7	0	-0.716668	1.890049	0.000568
8	7	0	1.297662	0.647033	-0.000659
9	7	0	1.609645	-1.594813	0.000251
10	7	0	-2.722046	0.506366	0.000050
11	7	0	-1.681250	-1.567378	0.000023
12	6	0	-0.731636	-0.591103	-0.000372
13	1	0	3.745655	-1.499138	0.000911
14	1	0	3.382827	1.241112	-0.000779
15	1	0	1.180291	2.742128	-0.000024
16	1	0	-3.794500	-1.329871	-0.000042

1,N^6-ethenoadenine: C8H C2 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.908052139 A.U.
Zero-point correction= .108203
(Hartree/Particle)
Thermal correction to Energy= .116039
Thermal correction to Enthalpy= .116983
Thermal correction to Gibbs Free Energy= .075158

```
 Sum of electronic and zero-point Energies=          -542.799849
 Sum of electronic and thermal Energies=             -542.792013
 Sum of electronic and thermal Enthalpies=           -542.791069
 Sum of electronic and thermal Free Energies=        -542.832895

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.816             31.241             88.029

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.876141   -0.887200   -0.000011
    2          6             0        2.669240    0.482259   -0.000102
    3          6             0        0.760932   -0.599626    0.000022
    4          6             0        0.644141    2.018212   -0.000159
    5          6             0       -1.338814    0.745549   -0.000036
    6          6             0       -2.829283   -0.852096    0.000149
    7          7             0       -0.670972    1.955000   -0.000120
    8          7             0        1.315872    0.666744   -0.000079
    9          7             0        1.681862   -1.562758    0.000068
   10          7             0       -2.631966    0.585345    0.000039
   11          7             0       -1.545896   -1.562589    0.000137
   12          6             0       -0.678705   -0.601695    0.000051
   13          1             0        3.819590   -1.420245    0.000000
   14          1             0        3.338910    1.330169   -0.000181
   15          1             0       -3.411390   -1.157322   -0.883434
   16          1             0       -3.411323   -1.157209    0.883816
 ---------------------------------------------------------------------
```

1,N^6-ethenoadenine: C8H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.874977550     A.U.
 Zero-point correction=                           0.107982
(Hartree/Particle)
 Thermal correction to Energy=                    0.115821
 Thermal correction to Enthalpy=                  0.116765
 Thermal correction to Gibbs Free Energy=         0.074941
 Sum of electronic and zero-point Energies=          -542.766996
 Sum of electronic and thermal Energies=             -542.759157
 Sum of electronic and thermal Enthalpies=           -542.758213
 Sum of electronic and thermal Free Energies=        -542.800037

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.679             31.291             88.026

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z

---------------------------------------------------------------------
```

1	6	0	2.987176	-1.052106	-0.000187
2	6	0	2.764976	0.317651	0.000016
3	6	0	0.765250	-0.670922	-0.000006
4	6	0	0.697880	1.781154	-0.000151
5	6	0	-1.312554	0.745580	0.000034
6	6	0	-2.842251	-0.795837	0.000159
7	7	0	-0.597145	1.934336	-0.000066
8	7	0	1.379603	0.600363	-0.000105
9	7	0	1.661308	-1.629881	-0.000053
10	7	0	-2.603956	0.643042	0.000114
11	7	0	-1.586559	-1.539639	0.000124
12	6	0	-0.674541	-0.614985	0.000068
13	1	0	3.461613	1.149207	0.000051
14	1	0	-3.437622	-1.071236	-0.883601
15	1	0	-3.437537	-1.071189	0.883992
16	1	0	1.325171	2.672463	-0.000136

1,N^6-ethenoadenine: C8H C12 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.909205488 A.U.
Zero-point correction= 0.109379
(Hartree/Particle)
Thermal correction to Energy= 0.116966
Thermal correction to Enthalpy= 0.117910
Thermal correction to Gibbs Free Energy= 0.076577
Sum of electronic and zero-point Energies= -542.799827
Sum of electronic and thermal Energies= -542.792240
Sum of electronic and thermal Enthalpies= -542.791296
Sum of electronic and thermal Free Energies= -542.832629

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.397	30.389	86.993

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.892395	-0.872034	-0.000206
2	6	0	2.793399	0.531588	0.000192
3	6	0	0.766358	-0.628774	0.000045
4	6	0	0.666482	1.813387	-0.000156
5	6	0	-1.323466	0.726124	-0.000018
6	6	0	-2.830302	-0.839551	0.000068
7	7	0	-0.628737	1.929720	-0.000134
8	7	0	1.383590	0.643821	-0.000044
9	7	0	1.696214	-1.566550	0.000090
10	7	0	-2.612535	0.603229	-0.000016
11	7	0	-1.562129	-1.564331	0.000135
12	6	0	-0.664009	-0.621419	0.000074
13	1	0	-3.424223	-1.121893	-0.883446
14	1	0	-3.424235	-1.121776	0.883611
15	1	0	3.818392	-1.438195	-0.000242

16	1	0	1.290104	2.704705	-0.000127

1,N^6-ethenoadenine: C8H N7 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.851912194 A.U.
Zero-point correction= 0.135757
(Hartree/Particle)
Thermal correction to Energy= 0.143608
Thermal correction to Enthalpy= 0.144552
Thermal correction to Gibbs Free Energy= 0.102809
Sum of electronic and zero-point Energies= -543.716155
Sum of electronic and thermal Energies= -543.708305
Sum of electronic and thermal Enthalpies= -543.707360
Sum of electronic and thermal Free Energies= -543.749103

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.115	32.194	87.855

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.845692	-0.999215	-0.000179
2	6	0	2.721038	0.390786	0.000100
3	6	0	0.748009	-0.606828	0.000042
4	6	0	0.674289	1.867992	-0.000242
5	6	0	-1.314204	0.768232	-0.000027
6	6	0	-2.913182	-0.743476	0.000156
7	7	0	-0.605197	1.955806	-0.000193
8	7	0	1.378472	0.646127	-0.000098
9	7	0	1.629596	-1.598686	0.000083
10	7	0	-2.601206	0.652942	0.000024
11	7	0	-1.612660	-1.455765	0.000194
12	6	0	-0.654944	-0.557940	0.000088
13	1	0	-3.497596	-1.010984	-0.890918
14	1	0	-3.497551	-1.010820	0.891309
15	1	0	3.761919	-1.574060	-0.000279
16	1	0	3.462345	1.178224	0.000152
17	1	0	-1.484867	-2.464816	0.000281
18	1	0	1.292527	2.762181	-0.000242

1,N^6-ethenoadenine: C8H N9 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.850629597 A.U.
Zero-point correction= 0.135662
(Hartree/Particle)
Thermal correction to Energy= 0.143550
Thermal correction to Enthalpy= 0.144494

```
 Thermal correction to Gibbs Free Energy=         0.102683
 Sum of electronic and zero-point Energies=           -543.714968
 Sum of electronic and thermal Energies=              -543.707080
 Sum of electronic and thermal Enthalpies=            -543.706136
 Sum of electronic and thermal Free Energies=         -543.747946

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.079             32.289             87.998

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        2.895543   -0.942922    0.000123
    2          6             0        2.751683    0.417446   -0.000133
    3          6             0        0.770960   -0.641039    0.000031
    4          6             0        0.673451    1.817462   -0.000073
    5          6             0       -1.282454    0.728206   -0.000028
    6          6             0       -2.846722   -0.917092    0.000042
    7          7             0       -0.636170    1.910772   -0.000092
    8          7             0        1.371848    0.645793   -0.000033
    9          7             0        1.666762   -1.584765    0.000120
   10          7             0       -2.582296    0.534045   -0.000039
   11          7             0       -1.560048   -1.557505    0.000086
   12          6             0       -0.668805   -0.620881    0.000028
   13          1             0       -3.421660   -1.204685   -0.890803
   14          1             0       -3.421647   -1.204576    0.890932
   15          1             0        3.815149   -1.511205    0.000208
   16          1             0        3.465755    1.228324   -0.000262
   17          1             0       -3.280966    1.273881   -0.000121
   18          1             0        1.260761    2.732806   -0.000185
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: C8H N10 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.847395565     A.U.
 Zero-point correction=                           0.135648
(Hartree/Particle)
 Thermal correction to Energy=                    0.143491
 Thermal correction to Enthalpy=                  0.144435
 Thermal correction to Gibbs Free Energy=         0.102698
 Sum of electronic and zero-point Energies=           -543.711748
 Sum of electronic and thermal Energies=              -543.703905
 Sum of electronic and thermal Enthalpies=            -543.702960
 Sum of electronic and thermal Free Energies=         -543.744697

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.042             32.254             87.843

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	2.906399	-0.866720	-0.000115
2	6	0	2.685016	0.479548	0.000004
3	6	0	0.701607	-0.558581	0.000007
4	6	0	0.555121	1.887174	-0.000115
5	6	0	-1.407110	0.732376	0.000000
6	6	0	-2.864645	-0.869943	0.000126
7	7	0	-0.717303	1.941954	-0.000078
8	7	0	1.306672	0.659726	-0.000064
9	7	0	1.666918	-1.485229	-0.000005
10	7	0	-2.686445	0.567351	0.000070
11	7	0	-1.573739	-1.560955	0.000102
12	6	0	-0.734354	-0.582763	0.000054
13	1	0	-3.448012	-1.180655	-0.880035
14	1	0	-3.447937	-1.180589	0.880361
15	1	0	3.828395	-1.428760	-0.000179
16	1	0	3.376139	1.309409	0.000028
17	1	0	1.494012	-2.487113	0.000016
18	1	0	1.172465	2.781238	-0.000126

1,N^6-ethenoadenine: C8H N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.833597548 A.U.
Zero-point correction= 0.135377
(Hartree/Particle)
Thermal correction to Energy= 0.143275
Thermal correction to Enthalpy= 0.144219
Thermal correction to Gibbs Free Energy= 0.102423
Sum of electronic and zero-point Energies= -543.698221
Sum of electronic and thermal Energies= -543.690323
Sum of electronic and thermal Enthalpies= -543.689379
Sum of electronic and thermal Free Energies= -543.731175

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.906	32.500	87.967

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.872960	-0.967340	-0.000014
2	6	0	2.745985	0.386833	-0.000195
3	6	0	0.736433	-0.678253	-0.000030
4	6	0	0.706543	1.797529	0.000014
5	6	0	-1.376959	0.663793	0.000022
6	6	0	-2.869230	-0.869331	0.000097
7	7	0	-0.614950	1.848050	0.000030
8	7	0	1.358690	0.631155	-0.000031
9	7	0	1.631144	-1.606380	0.000023
10	7	0	-2.651570	0.578069	0.000017

11	7	0	-1.601088	-1.581207	0.000060
12	6	0	-0.709690	-0.649069	-0.000006
13	1	0	-3.461302	-1.155595	-0.881490
14	1	0	-3.461227	-1.155527	0.881759
15	1	0	3.786536	-1.545531	0.000017
16	1	0	3.467182	1.191232	-0.000314
17	1	0	-1.094544	2.747790	0.000032
18	1	0	1.271513	2.724850	-0.000029

1,N^6-ethenoadenine: C8H N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.749783859 A.U.
Zero-point correction= 0.133011
(Hartree/Particle)
Thermal correction to Energy= 0.141202
Thermal correction to Enthalpy= 0.142146
Thermal correction to Gibbs Free Energy= 0.099684
Sum of electronic and zero-point Energies= -543.616775
Sum of electronic and thermal Energies= -543.608584
Sum of electronic and thermal Enthalpies= -543.607639
Sum of electronic and thermal Free Energies= -543.650101

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.606	33.408	89.368

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.812347	-0.954682	-0.288948
2	6	0	-2.764034	0.305981	0.173300
3	6	0	-0.681742	-0.732621	0.091347
4	6	0	-0.654463	1.846658	-0.103783
5	6	0	1.354272	0.724914	-0.108965
6	6	0	2.923268	-0.752688	0.058424
7	7	0	0.578689	1.874676	-0.309339
8	7	0	-1.357909	0.584291	0.500214
9	7	0	-1.535997	-1.564831	-0.345307
10	7	0	2.633360	0.658498	-0.143932
11	7	0	1.681438	-1.516504	0.200449
12	6	0	0.764400	-0.623157	0.097566
13	1	0	3.550783	-0.892316	0.949744
14	1	0	3.497495	-1.142308	-0.795017
15	1	0	-3.685049	-1.508181	-0.610159
16	1	0	-3.524549	1.048296	0.371278
17	1	0	-1.264122	0.689331	1.525447
18	1	0	-1.347744	2.665833	-0.269535

1,N^6-ethenoadenine: NEUTRAL C4H
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.471274851     A.U.
 Zero-point correction=                           0.122670
(Hartree/Particle)
 Thermal correction to Energy=                    0.130341
 Thermal correction to Enthalpy=                  0.131285
 Thermal correction to Gibbs Free Energy=         0.089756
 Sum of electronic and zero-point Energies=           -543.348605
 Sum of electronic and thermal Energies=              -543.340934
 Sum of electronic and thermal Enthalpies=            -543.339990
 Sum of electronic and thermal Free Energies=         -543.381519

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  81.790             30.981            87.405
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.871653	-0.875511	0.005455
2	6	0	2.659780	0.483346	-0.081059
3	6	0	0.745291	-0.636396	0.102716
4	6	0	0.513729	1.810727	-0.206274
5	6	0	-1.385350	0.656891	0.412606
6	6	0	-2.787963	-0.859607	-0.220888
7	7	0	-0.751543	1.868062	-0.076103
8	7	0	1.291869	0.647999	-0.006869
9	7	0	1.685133	-1.559738	0.107960
10	7	0	-2.773913	0.401132	0.046549
11	7	0	-1.548799	-1.572902	-0.220057
12	6	0	-0.692781	-0.655782	0.100220
13	1	0	-3.696921	-1.401223	-0.463005
14	1	0	-1.402754	0.755376	1.515877
15	1	0	1.080564	2.689045	-0.509025
16	1	0	3.334977	1.320433	-0.184157
17	1	0	3.818743	-1.397514	0.003304

1,N^6-ethenoadenine: C4H C8 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) = -542.852902052     A.U.
 Zero-point correction=                           0.106637
(Hartree/Particle)
 Thermal correction to Energy=                    0.114726
 Thermal correction to Enthalpy=                  0.115670
 Thermal correction to Gibbs Free Energy=         0.073393
 Sum of electronic and zero-point Energies=           -542.746265
 Sum of electronic and thermal Energies=              -542.738176
 Sum of electronic and thermal Enthalpies=            -542.737232
 Sum of electronic and thermal Free Energies=         -542.779510
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.992	32.289	88.981

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.869428	-0.805343	0.040008
2	6	0	2.619416	0.535477	-0.137464
3	6	0	0.727387	-0.629049	0.131672
4	6	0	0.420473	1.791643	-0.228660
5	6	0	-1.454981	0.588424	0.464693
6	6	0	-2.928584	-0.957652	-0.299449
7	7	0	-0.835792	1.820830	-0.008645
8	7	0	1.240066	0.655440	-0.067073
9	7	0	1.704563	-1.522501	0.198015
10	7	0	-2.847366	0.288620	0.063714
11	7	0	-1.506774	-1.593323	-0.360343
12	6	0	-0.723459	-0.691181	0.106133
13	1	0	-1.510051	0.691764	1.563311
14	1	0	0.951751	2.680744	-0.569282
15	1	0	3.263499	1.387567	-0.302107
16	1	0	3.833840	-1.297447	0.066803

1,N^6-ethenoadenine: C4H C4 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.990051456 A.U.
Zero-point correction= 0.110312
(Hartree/Particle)
Thermal correction to Energy= 0.117700
Thermal correction to Enthalpy= 0.118645
Thermal correction to Gibbs Free Energy= 0.077813
Sum of electronic and zero-point Energies= -542.879739
Sum of electronic and thermal Energies= -542.872351
Sum of electronic and thermal Enthalpies= -542.871407
Sum of electronic and thermal Free Energies= -542.912238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.858	30.228	85.937

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.814776	-0.943070	0.000059
2	6	0	-2.673253	0.426515	0.000031
3	6	0	-0.685936	-0.627258	-0.000018
4	6	0	-0.583041	1.832615	0.000081
5	6	0	1.372269	0.687617	0.000019
6	6	0	2.824345	-0.839895	-0.000123
7	7	0	0.716548	1.889841	0.000063

8	7	0	-1.298069	0.647107	0.000049
9	7	0	-1.610026	-1.594753	0.000002
10	7	0	2.722058	0.506230	-0.000155
11	7	0	1.681983	-1.566834	0.000016
12	6	0	0.731326	-0.590827	-0.000037
13	1	0	-1.180334	2.741671	0.000108
14	1	0	-3.382413	1.241696	0.000066
15	1	0	-3.745474	-1.499600	0.000085
16	1	0	3.795153	-1.329088	-0.000151

1,N^6-ethenoadenine: C4H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.857169861     A.U.
 Zero-point correction=                           0.108063
(Hartree/Particle)
 Thermal correction to Energy=                    0.115784
 Thermal correction to Enthalpy=                  0.116728
 Thermal correction to Gibbs Free Energy=         0.075106
 Sum of electronic and zero-point Energies=           -542.749107
 Sum of electronic and thermal Energies=              -542.741386
 Sum of electronic and thermal Enthalpies=            -542.740442
 Sum of electronic and thermal Free Energies=         -542.782064

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.656             30.890            87.601
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.990119	-0.989986	0.001119
2	6	0	2.711241	0.383626	-0.054807
3	6	0	0.765473	-0.671283	0.090758
4	6	0	0.600754	1.772011	-0.200664
5	6	0	-1.327350	0.680786	0.386818
6	6	0	-2.761143	-0.821515	-0.197023
7	7	0	-0.676120	1.884847	-0.100231
8	7	0	1.337592	0.618480	0.022397
9	7	0	1.706425	-1.604298	0.069484
10	7	0	-2.730594	0.452639	0.039638
11	7	0	-1.565659	-1.564933	-0.187956
12	6	0	-0.655763	-0.654676	0.083604
13	1	0	1.191740	2.640070	-0.494624
14	1	0	3.382754	1.231898	-0.140234
15	1	0	-3.691086	-1.341248	-0.419339
16	1	0	-1.324897	0.768348	1.492044

1,N^6-ethenoadenine: C4H C12 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.892407183     A.U.
 Zero-point correction=                           0.109383
(Hartree/Particle)
 Thermal correction to Energy=                    0.116888
 Thermal correction to Enthalpy=                  0.117832
 Thermal correction to Gibbs Free Energy=         0.076632
 Sum of electronic and zero-point Energies=           -542.783025
 Sum of electronic and thermal Energies=              -542.775519
 Sum of electronic and thermal Enthalpies=            -542.774575
 Sum of electronic and thermal Free Energies=         -542.815775

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.348             30.110            86.713
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.889582	-0.815637	-0.005181
2	6	0	2.733845	0.596107	-0.083622
3	6	0	0.765650	-0.626997	0.096624
4	6	0	0.567671	1.805314	-0.195959
5	6	0	-1.342561	0.663871	0.390112
6	6	0	-2.742576	-0.869335	-0.202005
7	7	0	-0.709910	1.878869	-0.097220
8	7	0	1.345800	0.666068	0.012596
9	7	0	1.734287	-1.541105	0.076180
10	7	0	-2.738907	0.407432	0.028128
11	7	0	-1.537376	-1.591197	-0.180434
12	6	0	-0.643762	-0.657995	0.093518
13	1	0	1.151641	2.678018	-0.481523
14	1	0	-3.661705	-1.405960	-0.431482
15	1	0	-1.353243	0.757759	1.494785
16	1	0	3.838962	-1.342258	-0.017464

1,N^6-ethenoadenine: C4H N7 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.829740736     A.U.
Zero-point correction=                           0.135459
(Hartree/Particle)
 Thermal correction to Energy=                    0.143242
 Thermal correction to Enthalpy=                  0.144186
 Thermal correction to Gibbs Free Energy=         0.102555
 Sum of electronic and zero-point Energies=           -543.694282
 Sum of electronic and thermal Energies=              -543.686500
 Sum of electronic and thermal Enthalpies=            -543.685555
 Sum of electronic and thermal Free Energies=         -543.727186
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.885	32.042	87.620

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.854560	-0.940500	-0.021626
2	6	0	2.679942	0.450701	-0.078131
3	6	0	0.751581	-0.608012	0.109115
4	6	0	0.581838	1.855584	-0.177300
5	6	0	-1.351724	0.713369	0.373824
6	6	0	-2.836712	-0.778772	-0.211369
7	7	0	-0.684327	1.907443	-0.075843
8	7	0	1.342729	0.665524	0.015263
9	7	0	1.667948	-1.574556	0.077338
10	7	0	-2.735182	0.477143	-0.026264
11	7	0	-1.587133	-1.488777	-0.107013
12	6	0	-0.641805	-0.596146	0.131973
13	1	0	1.161056	2.734473	-0.449966
14	1	0	-3.744222	-1.327130	-0.437959
15	1	0	-1.409727	0.815080	1.479423
16	1	0	3.790228	-1.482649	-0.053641
17	1	0	3.393625	1.255691	-0.192039
18	1	0	-1.445284	-2.480239	-0.289100

1,N^6-ethenoadenine: C4H N9 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.834279072 A.U.
Zero-point correction= 0.135660
(Hartree/Particle)
Thermal correction to Energy= 0.143501
Thermal correction to Enthalpy= 0.144445
Thermal correction to Gibbs Free Energy= 0.102698
Sum of electronic and zero-point Energies= -543.698620
Sum of electronic and thermal Energies= -543.690779
Sum of electronic and thermal Enthalpies= -543.689834
Sum of electronic and thermal Free Energies= -543.731581

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.048	32.051	87.863

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.875423	-0.904736	-0.020551
2	6	0	2.676853	0.476882	-0.083058
3	6	0	0.760615	-0.623843	0.117510

4	6	0	0.562588	1.832659	-0.200153
5	6	0	-1.318182	0.678183	0.425663
6	6	0	-2.709444	-0.964245	-0.238447
7	7	0	-0.707113	1.878077	-0.085295
8	7	0	1.329580	0.666218	0.021130
9	7	0	1.698297	-1.563123	0.084227
10	7	0	-2.670808	0.343188	-0.018288
11	7	0	-1.516680	-1.601968	-0.162356
12	6	0	-0.644623	-0.647434	0.137959
13	1	0	1.122523	2.712247	-0.508879
14	1	0	-3.630845	-1.484715	-0.479834
15	1	0	-1.367901	0.793028	1.525594
16	1	0	3.819660	-1.431712	-0.051062
17	1	0	3.371720	1.296842	-0.204733
18	1	0	-3.467469	0.972787	0.009451

1,N^6-ethenoadenine: C4H N10 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.825127668     A.U.
 Zero-point correction=                           0.135648
(Hartree/Particle)
 Thermal correction to Energy=                    0.143515
 Thermal correction to Enthalpy=                  0.144459
 Thermal correction to Gibbs Free Energy=         0.102606
 Sum of electronic and zero-point Energies=           -543.689480
 Sum of electronic and thermal Energies=              -543.681612
 Sum of electronic and thermal Enthalpies=            -543.680668
 Sum of electronic and thermal Free Energies=         -543.722522

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.057             32.194             88.089
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.920818	-0.789982	-0.024376
2	6	0	2.644162	0.546408	-0.100684
3	6	0	0.711654	-0.556428	0.124880
4	6	0	0.447297	1.859808	-0.192726
5	6	0	-1.448193	0.664144	0.417459
6	6	0	-2.795917	-0.904878	-0.246780
7	7	0	-0.810270	1.871831	-0.063544
8	7	0	1.267844	0.678125	-0.004446
9	7	0	1.711432	-1.448478	0.104174
10	7	0	-2.809381	0.356833	0.005711
11	7	0	-1.518226	-1.577178	-0.205015
12	6	0	-0.720302	-0.627243	0.139159
13	1	0	1.011342	2.740872	-0.487707
14	1	0	-3.677539	-1.478971	-0.508504
15	1	0	-1.524274	0.793312	1.516401
16	1	0	3.863110	-1.316899	-0.047250

17	1	0	3.300700	1.396488	-0.214542
18	1	0	1.579759	-2.453697	0.181848

1,N^6-ethenoadenine: C4H N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.814622150 A.U.
Zero-point correction= 0.135659
(Hartree/Particle)
Thermal correction to Energy= 0.143575
Thermal correction to Enthalpy= 0.144519
Thermal correction to Gibbs Free Energy= 0.102596
Sum of electronic and zero-point Energies= -543.678964
Sum of electronic and thermal Energies= -543.671048
Sum of electronic and thermal Enthalpies= -543.670103
Sum of electronic and thermal Free Energies= -543.712027

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.094	32.269	88.235

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.894084	-0.871823	-0.013077
2	6	0	2.697876	0.473537	-0.109133
3	6	0	0.753437	-0.667559	0.139907
4	6	0	0.578116	1.767111	-0.206202
5	6	0	-1.417583	0.586492	0.484370
6	6	0	-2.777665	-0.894667	-0.269524
7	7	0	-0.723193	1.763209	-0.059387
8	7	0	1.307684	0.655617	-0.001366
9	7	0	1.691126	-1.559221	0.121276
10	7	0	-2.769949	0.360765	0.034162
11	7	0	-1.527565	-1.598838	-0.238387
12	6	0	-0.687196	-0.697838	0.138441
13	1	0	1.082412	2.682715	-0.503349
14	1	0	-3.672884	-1.427767	-0.571057
15	1	0	-1.454451	0.710365	1.580979
16	1	0	3.834048	-1.405792	-0.029503
17	1	0	3.377197	1.305610	-0.227422
18	1	0	-1.259460	2.612623	-0.232427

1,N^6-ethenoadenine: C4H N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.730720911 A.U.
Zero-point correction= 0.133083
(Hartree/Particle)

```
 Thermal correction to Energy=                    0.141353
 Thermal correction to Enthalpy=                  0.142297
 Thermal correction to Gibbs Free Energy=         0.099537
 Sum of electronic and zero-point Energies=           -543.597641
 Sum of electronic and thermal Energies=              -543.589370
 Sum of electronic and thermal Enthalpies=            -543.588426
 Sum of electronic and thermal Free Energies=         -543.631187

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  88.701             33.411             89.997

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        2.845667   -0.779858    0.360871
    2          6             0        2.704831    0.395837   -0.274538
    3          6             0        0.707391   -0.769284   -0.030213
    4          6             0        0.480242    1.812239   -0.171548
    5          6             0       -1.346107    0.536249    0.644606
    6          6             0       -2.856448   -0.691479   -0.316413
    7          7             0       -0.663058    1.770594    0.310454
    8          7             0        1.281331    0.522186   -0.618709
    9          7             0        1.616401   -1.467148    0.517278
   10          7             0       -2.745822    0.446147    0.265788
   11          7             0       -1.638092   -1.445302   -0.546197
   12          6             0       -0.741850   -0.716099    0.004508
   13          1             0        1.045611    2.714335   -0.389487
   14          1             0       -3.795918   -1.105171   -0.666062
   15          1             0       -1.305272    0.454258    1.743690
   16          1             0        3.756954   -1.218699    0.745717
   17          1             0        3.410611    1.150925   -0.591335
   18          1             0        1.170345    0.493386   -1.646455
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: NEUTRAL N10H
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.509072468     A.U.
  Zero-point correction=                           0.123808
(Hartree/Particle)
 Thermal correction to Energy=                    0.131508
 Thermal correction to Enthalpy=                  0.132452
 Thermal correction to Gibbs Free Energy=         0.091080
 Sum of electronic and zero-point Energies=           -543.385265
 Sum of electronic and thermal Energies=              -543.377564
 Sum of electronic and thermal Enthalpies=            -543.376620
 Sum of electronic and thermal Free Energies=         -543.417992

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.523             31.664             87.075

-------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.859510	-0.859897	0.000080
2	6	0	-2.652256	0.480456	0.000087
3	6	0	-0.633600	-0.546513	0.000052
4	6	0	-0.530748	1.868909	-0.000066
5	6	0	1.416894	0.701000	-0.000092
6	6	0	2.820616	-0.872833	-0.000150
7	1	0	-1.119312	2.780908	-0.000058
8	1	0	-3.782705	-1.418568	0.000098
9	1	0	-3.348664	1.303911	0.000092
10	1	0	3.780374	-1.377549	-0.000106
11	7	0	0.767485	1.900199	-0.000103
12	7	0	-1.263104	0.686065	0.000010
13	7	0	-1.622494	-1.488329	0.000091
14	7	0	2.743953	0.482038	0.000113
15	7	0	1.666833	-1.576695	-0.000057
16	6	0	0.749253	-0.576020	0.000006
17	1	0	-1.442298	-2.482263	0.000098

1,N^6-ethenoadenine: N10H C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.853012465 A.U.
Zero-point correction= 0.107248
(Hartree/Particle)
Thermal correction to Energy= 0.115615
Thermal correction to Enthalpy= 0.116559
Thermal correction to Gibbs Free Energy= 0.073680
Sum of electronic and zero-point Energies= -542.745764
Sum of electronic and thermal Energies= -542.737398
Sum of electronic and thermal Enthalpies= -542.736454
Sum of electronic and thermal Free Energies= -542.779332

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.549	33.213	90.246

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.835527	-0.826030	0.000015
2	6	0	-2.609953	0.514951	0.000065
3	6	0	-0.590234	-0.538378	0.000014
4	6	0	-0.465966	1.871278	-0.000013
5	6	0	1.487774	0.665643	-0.000047
6	6	0	2.939599	-1.007232	-0.000048
7	7	0	0.842543	1.875646	-0.000045
8	7	0	-1.219089	0.711477	0.000016
9	7	0	-1.614512	-1.475051	0.000019
10	7	0	2.790365	0.412216	0.000012
11	7	0	1.674556	-1.624799	-0.000014

12	6	0	0.779182	-0.614398	0.000003
13	1	0	-1.035167	2.797716	0.000003
14	1	0	-3.301937	1.342977	0.000101
15	1	0	-3.771338	-1.364796	0.000000
16	1	0	-1.437848	-2.467325	0.000045

1,N^6-ethenoadenine: N10H C2 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.911308335 A.U.
Zero-point correction= 0.108757
(Hartree/Particle)
Thermal correction to Energy= 0.116745
Thermal correction to Enthalpy= 0.117689
Thermal correction to Gibbs Free Energy= 0.075720
Sum of electronic and zero-point Energies= -542.802551
Sum of electronic and thermal Energies= -542.794563
Sum of electronic and thermal Enthalpies= -542.793619
Sum of electronic and thermal Free Energies= -542.835589

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.259	32.110	88.332

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.881155	-0.804422	-0.000056
2	6	0	2.626332	0.531070	-0.000026
3	6	0	0.648842	-0.517106	0.000030
4	6	0	0.573009	2.030503	-0.000118
5	6	0	-1.383777	0.712741	-0.000080
6	6	0	-2.803723	-0.870725	0.000184
7	7	0	-0.750825	1.928770	-0.000106
8	7	0	1.249935	0.721388	-0.000056
9	7	0	1.646732	-1.460218	0.000032
10	7	0	-2.726957	0.483994	0.000178
11	7	0	-1.656686	-1.579123	-0.000047
12	6	0	-0.733311	-0.560736	0.000037
13	1	0	3.285913	1.385454	-0.000042
14	1	0	3.814518	-1.347172	-0.000093
15	1	0	1.480674	-2.455561	0.000045
16	1	0	-3.767663	-1.374354	0.000261

1,N^6-ethenoadenine: N10H N10 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.990051456 A.U.

```
 Zero-point correction=                           0.110312
(Hartree/Particle)
 Thermal correction to Energy=                    0.117700
 Thermal correction to Enthalpy=                  0.118645
 Thermal correction to Gibbs Free Energy=         0.077813
 Sum of electronic and zero-point Energies=           -542.879739
 Sum of electronic and thermal Energies=              -542.872351
 Sum of electronic and thermal Enthalpies=            -542.871407
 Sum of electronic and thermal Free Energies=         -542.912238

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.858             30.228             85.937
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.814776	-0.943070	0.000059
2	6	0	-2.673253	0.426515	0.000031
3	6	0	-0.685936	-0.627258	-0.000018
4	6	0	-0.583041	1.832615	0.000081
5	6	0	1.372269	0.687617	0.000019
6	6	0	2.824345	-0.839895	-0.000123
7	7	0	0.716548	1.889841	0.000063
8	7	0	-1.298069	0.647107	0.000049
9	7	0	-1.610026	-1.594753	0.000002
10	7	0	2.722058	0.506230	-0.000155
11	7	0	1.681983	-1.566834	0.000016
12	6	0	0.731326	-0.590827	-0.000037
13	1	0	-3.382413	1.241696	0.000066
14	1	0	-3.745474	-1.499600	0.000085
15	1	0	3.795153	-1.329088	-0.000151
16	1	0	-1.180334	2.741671	0.000108

1,N^6-ethenoadenine: N10H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.938220480
 Zero-point correction=                           .110563
(Hartree/Particle)
 Thermal correction to Energy=                    .118074
 Thermal correction to Enthalpy=                  .119018
 Thermal correction to Gibbs Free Energy=         .077994
 Sum of electronic and zero-point Energies=           -542.827658
 Sum of electronic and thermal Energies=              -542.820146
 Sum of electronic and thermal Enthalpies=            -542.819202
 Sum of electronic and thermal Free Energies=         -542.860226

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  74.093             30.756             86.343
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.814776	-0.943070	0.000059
2	6	0	-2.673253	0.426515	0.000031
3	6	0	-0.685936	-0.627258	-0.000018
4	6	0	-0.583041	1.832615	0.000081
5	6	0	1.372269	0.687617	0.000019
6	6	0	2.824345	-0.839895	-0.000123
7	7	0	0.716548	1.889841	0.000063
8	7	0	-1.298069	0.647107	0.000049
9	7	0	-1.610026	-1.594753	0.000002
10	7	0	2.722058	0.506230	-0.000155
11	7	0	1.681983	-1.566834	0.000016
12	6	0	0.731326	-0.590827	-0.000037
13	1	0	-3.382413	1.241696	0.000066
14	1	0	-3.745474	-1.499600	0.000085
15	1	0	3.795153	-1.329088	-0.000151
16	1	0	-1.180334	2.741671	0.000108

1,N^6-ethenoadenine: N10H C12 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.938220339 A.U.
Zero-point correction= 0.110564
(Hartree/Particle)
Thermal correction to Energy= 0.118077
Thermal correction to Enthalpy= 0.119021
Thermal correction to Gibbs Free Energy= 0.077995
Sum of electronic and zero-point Energies= -542.827656
Sum of electronic and thermal Energies= -542.820144
Sum of electronic and thermal Enthalpies= -542.819200
Sum of electronic and thermal Free Energies= -542.860225

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.094	30.757	86.346

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.976197	-0.973193	0.000246
2	6	0	-2.718727	0.380685	0.000099
3	6	0	-0.675476	-0.574866	0.000004
4	6	0	-0.605711	1.826982	0.000165
5	6	0	1.366776	0.710946	-0.000032
6	6	0	2.810626	-0.829595	0.000286
7	7	0	0.698170	1.902803	0.000047
8	7	0	-1.317390	0.643533	0.000135
9	7	0	-1.658337	-1.508419	0.000051
10	7	0	2.713859	0.518677	-0.000712
11	7	0	1.666571	-1.554048	-0.000160

12	6	0	0.725418	-0.566245	-0.000092
13	1	0	-3.399259	1.221419	0.000099
14	1	0	3.779377	-1.321569	0.000140
15	1	0	-1.210674	2.729548	0.000171
16	1	0	-1.449815	-2.495507	0.000003

1,N^6-ethenoadenine: N10H N7 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.894986097     A.U.
 Zero-point correction=                           0.137070
(Hartree/Particle)
 Thermal correction to Energy=                    0.144942
 Thermal correction to Enthalpy=                  0.145887
 Thermal correction to Gibbs Free Energy=         0.104264
 Sum of electronic and zero-point Energies=           -543.757918
 Sum of electronic and thermal Energies=              -543.750045
 Sum of electronic and thermal Enthalpies=            -543.749101
 Sum of electronic and thermal Free Energies=         -543.790723

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.953             32.785            87.603
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.895786	-0.866172	0.000096
2	6	0	-2.689865	0.472930	0.000079
3	6	0	-0.673921	-0.554877	-0.000012
4	6	0	-0.585514	1.868082	0.000146
5	6	0	1.365221	0.723078	0.000034
6	6	0	2.909219	-0.736338	-0.000125
7	7	0	0.707399	1.910077	0.000103
8	7	0	-1.303467	0.675080	0.000094
9	7	0	-1.654093	-1.492350	-0.000013
10	7	0	2.719724	0.562681	-0.000268
11	7	0	1.737506	-1.462766	-0.000084
12	6	0	0.719569	-0.539406	-0.000048
13	1	0	3.874165	-1.227215	-0.000176
14	1	0	-1.181478	2.775303	0.000190
15	1	0	-1.509463	-2.493958	-0.000039
16	1	0	-3.814945	-1.432585	0.000124
17	1	0	-3.384541	1.298929	0.000118
18	1	0	1.673233	-2.473315	-0.000057

1,N^6-ethenoadenine: N10H N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.910604344     A.U.
```

```
 Zero-point correction=                           0.137756
(Hartree/Particle)
 Thermal correction to Energy=                    0.145447
 Thermal correction to Enthalpy=                  0.146392
 Thermal correction to Gibbs Free Energy=         0.105097
 Sum of electronic and zero-point Energies=           -543.772848
 Sum of electronic and thermal Energies=              -543.765157
 Sum of electronic and thermal Enthalpies=            -543.764213
 Sum of electronic and thermal Free Energies=         -543.805507

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.270             32.202             86.911
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.893791	-0.859027	0.000056
2	6	0	2.689938	0.482170	-0.000006
3	6	0	0.680315	-0.551793	0.000020
4	6	0	0.575958	1.868413	-0.000045
5	6	0	-1.333207	0.693700	-0.000037
6	6	0	-2.798637	-0.953980	0.000088
7	7	0	-0.724515	1.896500	-0.000064
8	7	0	1.301121	0.683475	-0.000010
9	7	0	1.653793	-1.483874	0.000053
10	7	0	-2.673410	0.417320	-0.000040
11	7	0	-1.641096	-1.583411	-0.000014
12	6	0	-0.718234	-0.572108	0.000004
13	1	0	-3.766409	-1.438143	0.000128
14	1	0	1.156304	2.784701	-0.000076
15	1	0	1.483084	-2.483383	0.000067
16	1	0	3.814324	-1.423222	0.000092
17	1	0	3.386362	1.306459	-0.000040
18	1	0	-3.424459	1.099283	-0.000128

1,N^6-ethenoadenine: N10H N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.870587468     A.U.
 Zero-point correction=                           0.137233
(Hartree/Particle)
 Thermal correction to Energy=                    0.145002
 Thermal correction to Enthalpy=                  0.145946
 Thermal correction to Gibbs Free Energy=         0.104525
 Sum of electronic and zero-point Energies=           -543.733354
 Sum of electronic and thermal Energies=              -543.725586
 Sum of electronic and thermal Enthalpies=            -543.724641
 Sum of electronic and thermal Free Energies=         -543.766062

                    E (Thermal)             CV                S
```

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	90.990	32.478	87.178

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.871356	-0.866053	0.000066
2	6	0	-2.673957	0.473907	0.000103
3	6	0	-0.648193	-0.576316	0.000041
4	6	0	-0.593071	1.846438	-0.000024
5	6	0	1.437048	0.636925	-0.000035
6	6	0	2.814019	-0.926605	-0.000190
7	7	0	0.739610	1.816154	-0.000049
8	7	0	-1.276490	0.678856	0.000024
9	7	0	-1.638338	-1.497873	0.000059
10	7	0	2.744199	0.440670	0.000024
11	7	0	1.650210	-1.612028	-0.000036
12	6	0	0.735920	-0.621918	0.000007
13	1	0	3.770598	-1.434163	-0.000163
14	1	0	-1.128030	2.785858	-0.000010
15	1	0	-1.471278	-2.498132	0.000069
16	1	0	-3.796077	-1.424196	0.000069
17	1	0	-3.371351	1.297102	0.000139
18	1	0	1.259344	2.694812	-0.000057

1,N^6-ethenoadenine: N10H N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.762114707 A.U.
Zero-point correction= 0.134360
(Hartree/Particle)
Thermal correction to Energy= 0.142610
Thermal correction to Enthalpy= 0.143554
Thermal correction to Gibbs Free Energy= 0.101002
Sum of electronic and zero-point Energies= -543.627755
Sum of electronic and thermal Energies= -543.619505
Sum of electronic and thermal Enthalpies= -543.618561
Sum of electronic and thermal Free Energies= -543.661113

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.489	33.699	89.558

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.767612	-0.919245	-0.302914
2	6	0	-2.684382	0.405707	-0.118931
3	6	0	-0.588117	-0.607137	0.214959
4	6	0	-0.491850	1.953190	-0.056432

5	6	0	1.431635	0.711986	0.005656
6	6	0	2.816970	-0.886120	-0.096381
7	7	0	0.756399	1.912398	-0.156115
8	7	0	-1.307136	0.685029	0.377227
9	7	0	-1.544576	-1.538420	-0.038019
10	7	0	2.700586	0.502109	-0.219231
11	7	0	1.707275	-1.567259	0.135073
12	6	0	0.766361	-0.569903	0.232056
13	1	0	3.783099	-1.364667	-0.200328
14	1	0	-1.123736	2.832806	-0.127712
15	1	0	-1.316056	-2.503117	-0.255272
16	1	0	-3.627628	-1.501193	-0.606513
17	1	0	-3.412854	1.200176	-0.169065
18	1	0	-1.388702	0.848126	1.398270

1,N^6-ethenoadenine: N10H N10 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.796783418 A.U.
Zero-point correction= 0.136564
(Hartree/Particle)
Thermal correction to Energy= 0.144524
Thermal correction to Enthalpy= 0.145468
Thermal correction to Gibbs Free Energy= 0.103419
Sum of electronic and zero-point Energies= -543.660219
Sum of electronic and thermal Energies= -543.652260
Sum of electronic and thermal Enthalpies= -543.651315
Sum of electronic and thermal Free Energies= -543.693364

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.690	32.325	88.499

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.924844	-0.728713	0.000063
2	6	0	-2.605061	0.568352	0.000046
3	6	0	-0.589661	-0.492909	0.000011
4	6	0	-0.460152	1.907710	0.000007
5	6	0	1.471518	0.713437	0.000021
6	6	0	2.815357	-0.917074	-0.000431
7	7	0	0.839773	1.913242	0.000022
8	7	0	-1.210708	0.740488	0.000022
9	7	0	-1.655672	-1.520856	0.000047
10	7	0	2.765389	0.457924	0.000050
11	7	0	1.657445	-1.599776	0.000092
12	6	0	0.755807	-0.591415	-0.000017
13	1	0	3.769390	-1.431918	-0.000122
14	1	0	-1.027620	2.833420	0.000031
15	1	0	-1.575050	-2.135809	0.826078
16	1	0	-3.872736	-1.245632	0.000086
17	1	0	-3.270277	1.422301	0.000057

18	1	0	-1.575083	-2.135835	-0.825968

1,N^6-ethenoadenine: NEUTRAL C2H
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.480881520 A.U.
Zero-point correction= 0.122831
(Hartree/Particle)
Thermal correction to Energy= 0.130728
Thermal correction to Enthalpy= 0.131672
Thermal correction to Gibbs Free Energy= 0.089580
Sum of electronic and zero-point Energies= -543.358050
Sum of electronic and thermal Energies= -543.350153
Sum of electronic and thermal Enthalpies= -543.349209
Sum of electronic and thermal Free Energies= -543.391301

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.033	31.293	88.591

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.822319	-0.971065	0.000225
2	6	0	2.653894	0.408635	-0.000523
3	6	0	0.712891	-0.643080	-0.000048
4	6	0	0.581417	1.900893	0.000109
5	6	0	-1.404710	0.686283	0.000506
6	6	0	-2.822958	-0.878339	0.000358
7	7	0	-0.854487	1.840133	0.000445
8	7	0	1.305255	0.616786	-0.000073
9	7	0	1.623906	-1.610843	-0.000246
10	7	0	-2.782692	0.422512	-0.000714
11	7	0	-1.597193	-1.602641	0.000057
12	6	0	-0.710772	-0.649546	0.000036
13	1	0	-3.755096	-1.433484	-0.000085
14	1	0	0.888646	2.472857	0.884242
15	1	0	0.888353	2.472954	-0.884066
16	1	0	3.755671	-1.518221	0.000446
17	1	0	3.366414	1.221579	-0.000803

1,N^6-ethenoadenine: C2H C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.869181380 A.U.
Zero-point correction= 0.107057
(Hartree/Particle)
Thermal correction to Energy= 0.115565
Thermal correction to Enthalpy= 0.116509
Thermal correction to Gibbs Free Energy= 0.073120

```
 Sum of electronic and zero-point Energies=          -542.762124
 Sum of electronic and thermal Energies=             -542.753616
 Sum of electronic and thermal Enthalpies=           -542.752672
 Sum of electronic and thermal Free Energies=        -542.796062

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.518             32.659             91.321

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0        2.830810   -0.901697    0.000288
    2          6             0        2.622449    0.463772   -0.000286
    3          6             0        0.700954   -0.642178   -0.000117
    4          6             0        0.498405    1.889972    0.000093
    5          6             0       -1.477759    0.627224    0.000095
    6          6             0       -3.032149   -0.958923    0.000071
    7          7             0       -0.934743    1.797471    0.000169
    8          7             0        1.256788    0.622870   -0.000051
    9          7             0        1.643024   -1.582003   -0.000344
   10          7             0       -2.833142    0.347059    0.000223
   11          7             0       -1.570023   -1.679465   -0.000125
   12          6             0       -0.749257   -0.702685   -0.000059
   13          1             0        0.812724    2.462925    0.884579
   14          1             0        0.812580    2.463041   -0.884367
   15          1             0        3.778880   -1.425778    0.000571
   16          1             0        3.301762    1.305382   -0.000398
 -----------------------------------------------------------------------
```

1,N^6-ethenoadenine: C2H C2 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.990052678     A.U.
 Zero-point correction=                           0.110307
(Hartree/Particle)
 Thermal correction to Energy=                    0.117694
 Thermal correction to Enthalpy=                  0.118638
 Thermal correction to Gibbs Free Energy=         0.077810
 Sum of electronic and zero-point Energies=          -542.879746
 Sum of electronic and thermal Energies=             -542.872358
 Sum of electronic and thermal Enthalpies=           -542.871414
 Sum of electronic and thermal Free Energies=        -542.912243

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.854             30.228             85.931

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0        2.814492   -0.943358    0.000200
```

2	6	0	2.673392	0.426354	-0.000230
3	6	0	0.686194	-0.626530	-0.000336
4	6	0	0.583136	1.832994	-0.000121
5	6	0	-1.371987	0.687652	0.000020
6	6	0	-2.824213	-0.840050	0.000363
7	7	0	-0.716675	1.889889	-0.000078
8	7	0	1.297843	0.646987	-0.000050
9	7	0	1.609681	-1.594853	0.000227
10	7	0	-2.722243	0.506260	0.000235
11	7	0	-1.681615	-1.566982	-0.000326
12	6	0	-0.731529	-0.590971	-0.000321
13	1	0	1.180149	2.742120	0.000523
14	1	0	3.745718	-1.499144	0.000467
15	1	0	3.383097	1.241040	0.001178
16	1	0	-3.794813	-1.329664	0.000316

1,N^6-ethenoadenine: C2H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.866746285     A.U.
 Zero-point correction=                           0.107784
(Hartree/Particle)
 Thermal correction to Energy=                    0.115041
 Thermal correction to Enthalpy=                  0.115985
 Thermal correction to Gibbs Free Energy=         0.075329
 Sum of electronic and zero-point Energies=           -542.758963
 Sum of electronic and thermal Energies=              -542.751706
 Sum of electronic and thermal Enthalpies=            -542.750761
 Sum of electronic and thermal Free Energies=         -542.791417

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.189             29.286             85.567
```

1	6	0	2.919207	-1.109329	-0.000207
2	6	0	2.681496	0.312145	-0.000140
3	6	0	0.726651	-0.681368	-0.000011
4	6	0	0.660406	1.877548	0.000008
5	6	0	-1.349836	0.708191	0.000223
6	6	0	-2.774771	-0.852604	0.000501
7	7	0	-0.783516	1.865879	0.000121
8	7	0	1.355346	0.586389	-0.000040
9	7	0	1.645939	-1.663235	-0.000035
10	7	0	-2.723397	0.469016	-0.000397
11	7	0	-1.609232	-1.590379	0.000029
12	6	0	-0.669713	-0.640290	0.000045
13	1	0	0.985010	2.444983	0.882968
14	1	0	3.402993	1.124423	-0.000228

15	1	0	-3.729577	-1.373846	-0.000043
16	1	0	0.984946	2.445001	-0.882966

1,N^6-ethenoadenine: C2H C12 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.902128025 A.U.
Zero-point correction= 0.109328
(Hartree/Particle)
Thermal correction to Energy= 0.117164
Thermal correction to Enthalpy= 0.118108
Thermal correction to Gibbs Free Energy= 0.075809
Sum of electronic and zero-point Energies= -542.792800
Sum of electronic and thermal Energies= -542.784964
Sum of electronic and thermal Enthalpies= -542.784020
Sum of electronic and thermal Free Energies= -542.826319

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.521	30.511	89.025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.829961	-0.926439	0.000155
2	6	0	2.721417	0.518195	-0.000380
3	6	0	0.728083	-0.632187	-0.000038
4	6	0	0.628758	1.905746	0.000015
5	6	0	-1.364947	0.690850	0.000293
6	6	0	-2.760472	-0.898834	0.000195
7	7	0	-0.816122	1.854431	0.000208
8	7	0	1.368814	0.635547	-0.000103
9	7	0	1.666921	-1.601521	-0.000109
10	7	0	-2.736320	0.422772	-0.000347
11	7	0	-1.581359	-1.615841	0.000122
12	6	0	-0.660939	-0.642838	0.000017
13	1	0	0.946654	2.480499	0.879003
14	1	0	-3.704927	-1.439210	0.000022
15	1	0	0.946478	2.480557	-0.878994
16	1	0	3.767084	-1.476524	0.000041

1,N^6-ethenoadenine: C2H N7 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.844773733 A.U.
Zero-point correction= 0.135669
(Hartree/Particle)
Thermal correction to Energy= 0.143662
Thermal correction to Enthalpy= 0.144606
Thermal correction to Gibbs Free Energy= 0.102478

```
 Sum of electronic and zero-point Energies=           -543.709105
 Sum of electronic and thermal Energies=              -543.701112
 Sum of electronic and thermal Enthalpies=            -543.700168
 Sum of electronic and thermal Free Energies=         -543.742296

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.149             32.376             88.667

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.805436   -1.034243    0.000257
    2          6             0       -2.677578    0.377621   -0.000126
    3          6             0       -0.721170   -0.616357   -0.000031
    4          6             0       -0.637740    1.934082    0.000170
    5          6             0        1.364831    0.729922    0.000267
    6          6             0        2.870026   -0.789703   -0.000059
    7          7             0        0.791146    1.871559    0.000318
    8          7             0       -1.360914    0.636506    0.000055
    9          7             0       -1.605272   -1.624135   -0.000137
   10          7             0        2.747784    0.489619   -0.000499
   11          7             0        1.629388   -1.494867   -0.000135
   12          6             0        0.661306   -0.579337   -0.000065
   13          1             0       -0.946567    2.504494   -0.884855
   14          1             0        3.803535   -1.340254   -0.000119
   15          1             0       -0.946703    2.504416    0.885195
   16          1             0       -3.727276   -1.601366    0.000397
   17          1             0       -3.431498    1.154095   -0.000174
   18          1             0        1.508160   -2.504069   -0.000130
 ---------------------------------------------------------------------
```

1,N^6-ethenoadenine: C2H N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.846967991     A.U.
 Zero-point correction=                           0.135612
(Hartree/Particle)
 Thermal correction to Energy=                    0.143665
 Thermal correction to Enthalpy=                  0.144609
 Thermal correction to Gibbs Free Energy=         0.102339
 Sum of electronic and zero-point Energies=           -543.711356
 Sum of electronic and thermal Energies=              -543.703303
 Sum of electronic and thermal Enthalpies=            -543.702359
 Sum of electronic and thermal Free Energies=         -543.744629

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.151             32.460             88.964

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

1	6	0	2.819914	-1.014344	0.000109
2	6	0	2.669931	0.397435	-0.000165
3	6	0	0.724827	-0.637607	0.000008
4	6	0	0.633527	1.931560	0.000002
5	6	0	-1.322452	0.697557	0.000071
6	6	0	-2.753653	-0.986260	0.000078
7	7	0	-0.801263	1.858185	0.000053
8	7	0	1.350897	0.635098	-0.000035
9	7	0	1.633072	-1.623375	0.000018
10	7	0	-2.681642	0.365619	-0.000127
11	7	0	-1.577454	-1.618127	0.000052
12	6	0	-0.663159	-0.632106	0.000013
13	1	0	0.939201	2.502038	0.885540
14	1	0	-3.705407	-1.506381	0.000002
15	1	0	0.939159	2.502067	-0.885531
16	1	0	3.751603	-1.565457	0.000171
17	1	0	3.411597	1.185856	-0.000270
18	1	0	-3.455028	1.022669	-0.000331

1,N^6-ethenoadenine: C2H N10 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.840734609 A.U.
Zero-point correction= 0.136067
(Hartree/Particle)
Thermal correction to Energy= 0.144102
Thermal correction to Enthalpy= 0.145046
Thermal correction to Gibbs Free Energy= 0.102852
Sum of electronic and zero-point Energies= -543.704667
Sum of electronic and thermal Energies= -543.696633
Sum of electronic and thermal Enthalpies= -543.695689
Sum of electronic and thermal Free Energies= -543.737883

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.425	32.479	88.806

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.882751	-0.878630	0.000123
2	6	0	-2.650091	0.471867	0.000059
3	6	0	-0.684135	-0.566408	0.000014
4	6	0	-0.513928	1.937218	0.000016
5	6	0	1.456483	0.688881	-0.000028
6	6	0	2.849126	-0.909666	0.000158
7	7	0	0.910570	1.842742	-0.000005
8	7	0	-1.281329	0.647177	0.000041
9	7	0	-1.653182	-1.499104	0.000022
10	7	0	2.822552	0.385301	-0.000185
11	7	0	1.576635	-1.604557	-0.000148
12	6	0	0.741265	-0.622573	-0.000045

13	1	0	-0.824752	2.501278	-0.887341
14	1	0	3.760807	-1.495622	-0.000137
15	1	0	-0.824715	2.501287	0.887379
16	1	0	-3.810110	-1.431918	0.000177
17	1	0	-3.342882	1.300649	0.000063
18	1	0	-1.480883	-2.500721	-0.000006

1,N^6-ethenoadenine: C2H N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.823629785     A.U.
 Zero-point correction=                           0.135364
(Hartree/Particle)
 Thermal correction to Energy=                    0.143706
 Thermal correction to Enthalpy=                  0.144651
 Thermal correction to Gibbs Free Energy=         0.100849
 Sum of electronic and zero-point Energies=           -543.688266
 Sum of electronic and thermal Energies=              -543.679923
 Sum of electronic and thermal Enthalpies=            -543.678979
 Sum of electronic and thermal Free Energies=         -543.722781

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.177             32.604             92.189
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.809029	-1.011213	0.000108
2	6	0	2.645916	0.391627	-0.000270
3	6	0	0.702451	-0.665746	-0.000103
4	6	0	0.653283	1.917085	0.000067
5	6	0	-1.430397	0.628535	0.000018
6	6	0	-2.781443	-0.953146	0.000744
7	7	0	-0.804284	1.784858	0.000044
8	7	0	1.316395	0.615067	-0.000047
9	7	0	1.624904	-1.632359	-0.000175
10	7	0	-2.741642	0.398014	-0.000061
11	7	0	-1.593467	-1.654252	-0.000178
12	6	0	-0.691093	-0.696055	-0.000077
13	1	0	0.949775	2.478400	0.892951
14	1	0	-3.728654	-1.482809	-0.000095
15	1	0	0.949742	2.478508	-0.892758
16	1	0	3.745691	-1.553633	0.000204
17	1	0	3.377649	1.189211	-0.000375
18	1	0	-1.354017	2.644524	0.000061

1,N^6-ethenoadenine: C2H N1 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.753854904     A.U.
 Zero-point correction=                           0.134208
(Hartree/Particle)
 Thermal correction to Energy=                    0.142452
 Thermal correction to Enthalpy=                  0.143396
 Thermal correction to Gibbs Free Energy=         0.100840
 Sum of electronic and zero-point Energies=           -543.619647
 Sum of electronic and thermal Energies=              -543.611404
 Sum of electronic and thermal Enthalpies=            -543.610459
 Sum of electronic and thermal Free Energies=         -543.653015

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.390             33.205             89.567
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.801054	-0.948725	-0.243005
2	6	0	-2.724572	0.314131	0.218985
3	6	0	-0.668096	-0.730329	0.086358
4	6	0	-0.620748	1.834301	-0.249359
5	6	0	1.406264	0.702774	-0.044300
6	6	0	2.902946	-0.793623	0.034501
7	7	0	0.793704	1.809294	-0.199813
8	7	0	-1.310724	0.583863	0.481454
9	7	0	-1.536230	-1.570268	-0.327625
10	7	0	2.788329	0.490682	-0.063552
11	7	0	1.677174	-1.572073	0.132267
12	6	0	0.769303	-0.662167	0.100108
13	1	0	-0.980383	1.804605	-1.282355
14	1	0	3.851142	-1.318731	0.049773
15	1	0	-1.017702	2.711675	0.265045
16	1	0	-3.688503	-1.494176	-0.536565
17	1	0	-3.472000	1.064912	0.434739
18	1	0	-1.162582	0.743057	1.490518

1,N^6-ethenoadenine: NEUTRAL C12H
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.494108953     A.U.
 Zero-point correction=                           0.123143
(Hartree/Particle)
 Thermal correction to Energy=                    0.130813
 Thermal correction to Enthalpy=                  0.131757
 Thermal correction to Gibbs Free Energy=         0.090266
 Sum of electronic and zero-point Energies=           -543.370966
 Sum of electronic and thermal Energies=              -543.363296
 Sum of electronic and thermal Enthalpies=            -543.362352
```

```
 Sum of electronic and thermal Free Energies=         -543.403843

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.086             30.865            87.326

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.731857   -1.052060    0.000097
    2          6             0       -2.688393    0.460505    0.000067
    3          6             0       -0.620927   -0.586706    0.000070
    4          6             0       -0.536609    1.833161   -0.000034
    5          6             0        1.423148    0.705613   -0.000088
    6          6             0        2.828382   -0.862445   -0.000278
    7          1             0       -1.127267    2.745139   -0.000027
    8          1             0       -3.653024   -1.627583    0.000133
    9          1             0       -3.159252    0.894698   -0.890986
   10          1             0        3.797696   -1.349345   -0.000126
   11          7             0        0.768170    1.896377   -0.000076
   12          7             0       -1.238084    0.658247    0.000031
   13          7             0       -1.573994   -1.612038    0.000062
   14          7             0        2.739800    0.504063    0.000135
   15          7             0        1.696404   -1.580690   -0.000044
   16          6             0        0.752084   -0.601292    0.000018
   17          1             0       -3.159198    0.894722    0.891136
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: C12H C8 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.852511794     A.U.
 Zero-point correction=                           0.106486
(Hartree/Particle)
 Thermal correction to Energy=                    0.114859
 Thermal correction to Enthalpy=                  0.115803
 Thermal correction to Gibbs Free Energy=         0.072305
 Sum of electronic and zero-point Energies=           -542.746026
 Sum of electronic and thermal Energies=              -542.737653
 Sum of electronic and thermal Enthalpies=            -542.736709
 Sum of electronic and thermal Free Energies=         -542.780207

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.075             32.258            91.549

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.717759   -1.017273   -0.000138
    2          6             0       -2.646378    0.500437   -0.000014
    3          6             0       -0.582609   -0.605292    0.000209
```

4	6	0	-0.476449	1.824464	0.000093
5	6	0	1.493344	0.672549	0.000212
6	6	0	2.961633	-0.991058	-0.000852
7	7	0	0.830227	1.878795	0.000238
8	7	0	-1.198606	0.667696	0.000089
9	7	0	-1.563528	-1.593766	0.000092
10	7	0	2.782204	0.459831	0.000013
11	7	0	1.720337	-1.622724	-0.000157
12	6	0	0.792687	-0.648696	0.000196
13	1	0	-1.057568	2.746041	0.000003
14	1	0	-3.117644	0.946517	-0.889651
15	1	0	-3.648450	-1.578350	-0.000357
16	1	0	-3.117578	0.946174	0.889843

1,N^6-ethenoadenine: C12H C2 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.904747384 A.U.
Zero-point correction= 0.108658
(Hartree/Particle)
Thermal correction to Energy= 0.116331
Thermal correction to Enthalpy= 0.117275
Thermal correction to Gibbs Free Energy= 0.075796
Sum of electronic and zero-point Energies= -542.796090
Sum of electronic and thermal Energies= -542.788416
Sum of electronic and thermal Enthalpies= -542.787472
Sum of electronic and thermal Free Energies= -542.828952

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.999	30.698	87.301

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.748882	-0.997424	0.000004
2	6	0	-2.667454	0.507624	0.000145
3	6	0	-0.633020	-0.557421	-0.000064
4	6	0	-0.610470	1.958837	0.000152
5	6	0	1.385776	0.722495	0.000108
6	6	0	2.819497	-0.839965	0.000195
7	7	0	0.746764	1.909468	0.000121
8	7	0	-1.222894	0.697074	0.000091
9	7	0	-1.598921	-1.582140	-0.000056
10	7	0	2.730120	0.513369	-0.000458
11	7	0	1.692353	-1.575517	-0.000128
12	6	0	0.740209	-0.589542	-0.000087
13	1	0	-3.130514	0.964681	-0.884997
14	1	0	-3.677254	-1.565257	-0.000024
15	1	0	-3.130433	0.964494	0.885429
16	1	0	3.792304	-1.327317	-0.000115

1,N^6-ethenoadenine: C12H C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.916264202     A.U.
 Zero-point correction=                           0.108892
(Hartree/Particle)
 Thermal correction to Energy=                    0.116555
 Thermal correction to Enthalpy=                  0.117499
 Thermal correction to Gibbs Free Energy=         0.076031
 Sum of electronic and zero-point Energies=           -542.807372
 Sum of electronic and thermal Energies=              -542.799709
 Sum of electronic and thermal Enthalpies=            -542.798765
 Sum of electronic and thermal Free Energies=         -542.840233

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.139             30.645             87.277


---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.844827   -1.173522    0.000070
    2          6             0       -2.736261    0.363963    0.000074
    3          6             0       -0.672637   -0.618564   -0.000007
    4          6             0       -0.598994    1.805985    0.000002
    5          6             0        1.369143    0.708417   -0.000011
    6          6             0        2.811150   -0.827558   -0.000382
    7          7             0        0.705512    1.904148   -0.000008
    8          7             0       -1.281679    0.624851    0.000025
    9          7             0       -1.596278   -1.650587    0.000054
   10          7             0        2.704812    0.531817    0.000066
   11          7             0        1.686993   -1.557684    0.000105
   12          6             0        0.722616   -0.585074   -0.000012
   13          1             0       -3.208366    0.793537   -0.892190
   14          1             0       -3.208315    0.793524    0.892371
   15          1             0        3.787721   -1.304226   -0.000314
   16          1             0       -1.207701    2.707462    0.000029
 ---------------------------------------------------------------------
```

1,N^6-ethenoadenine: C12H C12 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.916264202     A.U.
 Zero-point correction=                           0.108892
(Hartree/Particle)
 Thermal correction to Energy=                    0.116555
 Thermal correction to Enthalpy=                  0.117499
 Thermal correction to Gibbs Free Energy=         0.076031
 Sum of electronic and zero-point Energies=           -542.807372
 Sum of electronic and thermal Energies=              -542.799709
```

```
 Sum of electronic and thermal Enthalpies=            -542.798765
 Sum of electronic and thermal Free Energies=         -542.840233

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.139             30.645            87.277

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.844827   -1.173522    0.000070
    2          6             0       -2.736261    0.363963    0.000074
    3          6             0       -0.672637   -0.618564   -0.000007
    4          6             0       -0.598994    1.805985    0.000002
    5          6             0        1.369143    0.708417   -0.000011
    6          6             0        2.811150   -0.827558   -0.000382
    7          7             0        0.705512    1.904148   -0.000008
    8          7             0       -1.281679    0.624851    0.000025
    9          7             0       -1.596278   -1.650587    0.000054
   10          7             0        2.704812    0.531817    0.000066
   11          7             0        1.686993   -1.557684    0.000105
   12          6             0        0.722616   -0.585074   -0.000012
   13          1             0       -3.208366    0.793537   -0.892190
   14          1             0       -3.208315    0.793524    0.892371
   15          1             0        3.787721   -1.304226   -0.000314
   16          1             0       -1.207701    2.707462    0.000029
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: C12H N7 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.879425000     A.U.
 Zero-point correction=                           0.136495
(Hartree/Particle)
 Thermal correction to Energy=                    0.144297
 Thermal correction to Enthalpy=                  0.145241
 Thermal correction to Gibbs Free Energy=         0.103610
 Sum of electronic and zero-point Energies=          -543.742930
 Sum of electronic and thermal Energies=             -543.735128
 Sum of electronic and thermal Enthalpies=           -543.734184
 Sum of electronic and thermal Free Energies=        -543.775815

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.548             31.928            87.619

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.744752   -1.078196    0.000037
    2          6             0       -2.734334    0.430317    0.000110
    3          6             0       -0.660338   -0.561471    0.000026
```

4	6	0	-0.589157	1.848307	0.000085
5	6	0	1.375083	0.733180	-0.000062
6	6	0	2.895518	-0.746737	-0.000201
7	7	0	0.716903	1.909947	0.000030
8	7	0	-1.280418	0.666190	0.000072
9	7	0	-1.569047	-1.613028	-0.000026
10	7	0	2.722931	0.561167	0.000096
11	7	0	1.725379	-1.465776	-0.000148
12	6	0	0.715695	-0.540419	-0.000026
13	1	0	-3.209741	0.857027	-0.891788
14	1	0	3.859360	-1.240767	-0.000267
15	1	0	-1.178931	2.760205	0.000145
16	1	0	-3.651122	-1.676901	0.000035
17	1	0	-3.209659	0.856915	0.892107
18	1	0	1.633569	-2.475871	-0.000208

1,N^6-ethenoadenine: C12H N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.883632715     A.U.
  Zero-point correction=                           0.136612
(Hartree/Particle)
 Thermal correction to Energy=                    0.144367
 Thermal correction to Enthalpy=                  0.145312
 Thermal correction to Gibbs Free Energy=         0.103774
 Sum of electronic and zero-point Energies=           -543.747021
 Sum of electronic and thermal Energies=              -543.739265
 Sum of electronic and thermal Enthalpies=            -543.738321
 Sum of electronic and thermal Free Energies=         -543.779858

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.592             31.811             87.423
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.762270	-1.055392	-0.000009
2	6	0	-2.730992	0.452462	0.000047
3	6	0	-0.668201	-0.577433	0.000021
4	6	0	-0.580686	1.839845	0.000041
5	6	0	1.338867	0.697473	-0.000037
6	6	0	2.801857	-0.951293	-0.000162
7	7	0	0.731369	1.890848	0.000017
8	7	0	-1.272658	0.664328	0.000032
9	7	0	-1.595878	-1.608465	-0.000056
10	7	0	2.670948	0.430373	0.000188
11	7	0	1.657577	-1.588940	-0.000152
12	6	0	0.717807	-0.588967	-0.000016
13	1	0	-3.197708	0.886411	-0.892557
14	1	0	3.775729	-1.424493	-0.000157
15	1	0	-1.159395	2.758071	0.000078
16	1	0	-3.678050	-1.639742	-0.000020

17	1	0	-3.197660	0.886326	0.892718
18	1	0	3.419276	1.116257	0.000426

1,N^6-ethenoadenine: C12H N10 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.819715569 A.U.
Zero-point correction= 0.135637
(Hartree/Particle)
Thermal correction to Energy= 0.143572
Thermal correction to Enthalpy= 0.144516
Thermal correction to Gibbs Free Energy= 0.102523
Sum of electronic and zero-point Energies= -543.684079
Sum of electronic and thermal Energies= -543.676144
Sum of electronic and thermal Enthalpies= -543.675199
Sum of electronic and thermal Free Energies= -543.717192

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.093	32.116	88.382

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.786835	-0.975747	0.000071
2	6	0	-2.678960	0.519360	0.000096
3	6	0	-0.583350	-0.523325	0.000041
4	6	0	-0.486584	1.868796	0.000011
5	6	0	1.470604	0.716456	-0.000069
6	6	0	2.843914	-0.882209	-0.000310
7	7	0	0.820961	1.899591	-0.000033
8	7	0	-1.217039	0.703754	0.000041
9	7	0	-1.594664	-1.494868	0.000030
10	7	0	2.774860	0.481534	0.000126
11	7	0	1.685615	-1.588415	-0.000067
12	6	0	0.778936	-0.599830	-0.000002
13	1	0	-3.155614	0.955450	-0.889525
14	1	0	3.801944	-1.389306	-0.000100
15	1	0	-1.057257	2.792954	0.000037
16	1	0	-3.691991	-1.572625	0.000079
17	1	0	-3.155521	0.955387	0.889800
18	1	0	-1.376036	-2.494030	0.000003

1,N^6-ethenoadenine: C12H N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -543.847224306 A.U.
Zero-point correction= 0.136232
(Hartree/Particle)
Thermal correction to Energy= 0.144081

```
 Thermal correction to Enthalpy=                  0.145025
 Thermal correction to Gibbs Free Energy=         0.103305
 Sum of electronic and zero-point Energies=           -543.710992
 Sum of electronic and thermal Energies=              -543.703143
 Sum of electronic and thermal Enthalpies=            -543.702199
 Sum of electronic and thermal Free Energies=         -543.743919

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.412             32.094             87.807

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.742312   -1.068410    0.000071
    2          6             0       -2.715355    0.444049    0.000084
    3          6             0       -0.632852   -0.614502    0.000044
    4          6             0       -0.599427    1.818261    0.000005
    5          6             0        1.444121    0.641657   -0.000020
    6          6             0        2.820042   -0.925582   -0.000259
    7          7             0        0.736610    1.820901   -0.000015
    8          7             0       -1.251579    0.656591    0.000038
    9          7             0       -1.580350   -1.623150    0.000034
   10          7             0        2.736569    0.464279    0.000018
   11          7             0        1.680533   -1.616865   -0.000037
   12          6             0        0.738721   -0.639892    0.000004
   13          1             0       -3.179604    0.875947   -0.894134
   14          1             0        3.787758   -1.412522   -0.000169
   15          1             0       -1.141292    2.756000    0.000023
   16          1             0       -3.661420   -1.647429    0.000086
   17          1             0       -3.179524    0.875902    0.894367
   18          1             0        1.243963    2.706319   -0.000021
 -------------------------------------------------------------------
```

1,N^6-ethenoadenine: C12H N1 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -543.758001062     A.U.
 Zero-point correction=                           0.134596
(Hartree/Particle)
 Thermal correction to Energy=                    0.142738
 Thermal correction to Enthalpy=                  0.143682
 Thermal correction to Gibbs Free Energy=         0.101108
 Sum of electronic and zero-point Energies=           -543.623405
 Sum of electronic and thermal Energies=              -543.615263
 Sum of electronic and thermal Enthalpies=            -543.614319
 Sum of electronic and thermal Free Energies=         -543.656893

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.570             32.742             89.604

-------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.647873	-1.118770	-0.237163
2	6	0	-2.650596	0.401240	-0.257082
3	6	0	-0.578371	-0.666843	0.218505
4	6	0	-0.507171	1.926087	0.024359
5	6	0	1.426051	0.710779	0.000604
6	6	0	2.829340	-0.878375	-0.107519
7	7	0	0.744842	1.915796	-0.108250
8	7	0	-1.297363	0.670242	0.387452
9	7	0	-1.508363	-1.655855	0.025929
10	7	0	2.692210	0.533097	-0.201035
11	7	0	1.739041	-1.580675	0.084382
12	6	0	0.766139	-0.605371	0.179049
13	1	0	-2.652758	0.799287	-1.277992
14	1	0	3.810142	-1.328949	-0.204713
15	1	0	-1.125922	2.818101	-0.026142
16	1	0	-3.529824	-1.713994	-0.458284
17	1	0	-3.452294	0.865506	0.321362
18	1	0	-1.467028	0.769341	1.401892

9-Methyl-1,N^6-ethenoadenine: NEUTRAL N9CH3
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.842399736
 Zero-point correction=                           0.151944
(Hartree/Particle)
 Thermal correction to Energy=                    0.161388
 Thermal correction to Enthalpy=                  0.162333
 Thermal correction to Gibbs Free Energy=         0.116473
 Sum of electronic and zero-point Energies=           -582.690455
 Sum of electronic and thermal Energies=              -582.681011
 Sum of electronic and thermal Enthalpies=            -582.680067
 Sum of electronic and thermal Free Energies=         -582.725927
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.273	36.807	96.520

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.313621	-0.595086	0.000167
2	6	0	2.971092	0.735154	0.000046
3	6	0	1.172403	-0.607653	0.000000
4	6	0	0.703685	1.816537	-0.000096
5	6	0	-1.016221	0.385181	-0.000195
6	6	0	-2.266124	-1.415258	-0.000105
7	7	0	-0.592475	1.673942	-0.000206
8	7	0	1.580784	0.755398	-0.000017
9	7	0	2.212200	-1.417912	0.000167
10	7	0	-2.327564	-0.042834	-0.000283
11	7	0	-1.039169	-1.896854	-0.000110

12	6	0	-0.238870	-0.780436	-0.000080
13	1	0	-3.166719	-2.016589	-0.000083
14	1	0	1.144774	2.808541	-0.000116
15	1	0	3.555932	1.642738	-0.000004
16	1	0	4.313305	-1.009794	0.000256
17	6	0	-3.512205	0.801193	0.000447
18	1	0	-3.525473	1.436829	0.890630
19	1	0	-3.525897	1.437859	-0.888975
20	1	0	-4.396649	0.160451	0.000339

9-Methyl-1,N^6-ethenoadenine: N9CH3 C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -582.235300850 A.U.
Zero-point correction= 0.136880
(Hartree/Particle)
Thermal correction to Energy= 0.146256
Thermal correction to Enthalpy= 0.147200
Thermal correction to Gibbs Free Energy= 0.102039
Sum of electronic and zero-point Energies= -582.098421
Sum of electronic and thermal Energies= -582.089045
Sum of electronic and thermal Enthalpies= -582.088101
Sum of electronic and thermal Free Energies= -582.133262

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.777	36.932	95.049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.289183	-0.575442	-0.000125
2	6	0	2.934181	0.756250	-0.000095
3	6	0	1.138843	-0.601906	-0.000060
4	6	0	0.657446	1.816550	0.000004
5	6	0	-1.062594	0.363109	0.000026
6	6	0	-2.362449	-1.523064	0.000019
7	7	0	-0.642385	1.650392	0.000037
8	7	0	1.542213	0.759631	-0.000042
9	7	0	2.205464	-1.408063	-0.000099
10	7	0	-2.352560	-0.104689	0.000067
11	7	0	-1.052841	-1.922371	-0.000026
12	6	0	-0.266860	-0.807258	-0.000019
13	1	0	1.091354	2.812167	0.000007
14	1	0	3.507817	1.671825	-0.000106
15	1	0	4.296756	-0.976424	-0.000164
16	6	0	-3.535756	0.720591	0.000231
17	1	0	-3.576633	1.365693	0.889149
18	1	0	-3.576459	1.366253	-0.888282
19	1	0	-4.394041	0.043204	-0.000050

9-Methyl-1,N^6-ethenoadenine: N9CH3 C2 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.241848743     A.U.
  Zero-point correction=                           0.137166
(Hartree/Particle)
 Thermal correction to Energy=                    0.145827
 Thermal correction to Enthalpy=                  0.146772
 Thermal correction to Gibbs Free Energy=         0.103049
 Sum of electronic and zero-point Energies=           -582.104683
 Sum of electronic and thermal Energies=              -582.096021
 Sum of electronic and thermal Enthalpies=            -582.095077
 Sum of electronic and thermal Free Energies=         -582.138799

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.508             34.767             92.022
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        3.328956   -0.530497   -0.000105
    2          6             0        2.939420    0.787301   -0.000071
    3          6             0        1.187988   -0.577524   -0.000054
    4          6             0        0.728191    1.962480   -0.000008
    5          6             0       -0.983459    0.396750   -0.000002
    6          6             0       -2.256503   -1.414904   -0.000043
    7          7             0       -0.589109    1.694638    0.000016
    8          7             0        1.553860    0.784069   -0.000038
    9          7             0        2.244802   -1.385590   -0.000060
   10          7             0       -2.302824   -0.037639    0.000021
   11          7             0       -1.031256   -1.898589    0.000006
   12          6             0       -0.221523   -0.775620   -0.000029
   13          1             0       -3.163376   -2.009020   -0.000069
   14          1             0        3.481246    1.721110   -0.000074
   15          1             0        4.340179   -0.922175   -0.000139
   16          6             0       -3.468617    0.817706    0.000265
   17          1             0       -3.472984    1.462015    0.886408
   18          1             0       -3.472563    1.462960   -0.885181
   19          1             0       -4.367521    0.192737   -0.000274
 -------------------------------------------------------------------
```

9-Methyl-1,N^6-ethenoadenine: N9CH3 C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.204933296     A.U.
  Zero-point correction=                           0.136684
(Hartree/Particle)
 Thermal correction to Energy=                    0.146315
 Thermal correction to Enthalpy=                  0.147259
 Thermal correction to Gibbs Free Energy=         0.101057
 Sum of electronic and zero-point Energies=           -582.068249
 Sum of electronic and thermal Energies=              -582.058619
 Sum of electronic and thermal Enthalpies=            -582.057675
```

```
 Sum of electronic and thermal Free Energies=         -582.103876

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.814             37.169             97.239

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        3.463764   -0.656962   -0.000138
    2          6             0        3.035101    0.666412   -0.000111
    3          6             0        1.218743   -0.644593   -0.000074
    4          6             0        0.767807    1.785630   -0.000008
    5          6             0       -0.972045    0.389207    0.000011
    6          6             0       -2.251417   -1.402708    0.000009
    7          7             0       -0.549245    1.678276    0.000029
    8          7             0        1.630854    0.739378   -0.000057
    9          7             0        2.250674   -1.444776   -0.000109
   10          7             0       -2.295246   -0.026870    0.000032
   11          7             0       -1.031117   -1.894156   -0.000017
   12          6             0       -0.203382   -0.783524   -0.000031
   13          1             0       -3.162006   -1.991006    0.000010
   14          1             0        1.211948    2.778531   -0.000002
   15          1             0        3.601941    1.591531   -0.000119
   16          6             0       -3.458888    0.830568    0.000315
   17          1             0       -3.466963    1.473143    0.888338
   18          1             0       -3.466659    1.474039   -0.887053
   19          1             0       -4.357805    0.206624   -0.000153
 -------------------------------------------------------------------
```

9-Methyl-1,N^6-ethenoadenine: N9CH3 C12 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.234998172     A.U.
   Zero-point correction=                           0.137980
(Hartree/Particle)
 Thermal correction to Energy=                    0.147420
 Thermal correction to Enthalpy=                  0.148364
 Thermal correction to Gibbs Free Energy=         0.102415
 Sum of electronic and zero-point Energies=           -582.097018
 Sum of electronic and thermal Energies=              -582.087578
 Sum of electronic and thermal Enthalpies=            -582.086634
 Sum of electronic and thermal Free Energies=         -582.132583

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  92.508             36.373             96.709
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        3.350569   -0.496799   -0.000080
    2          6             0        3.048326    0.863858   -0.000048
    3          6             0        1.214297   -0.607835   -0.000050
```

4	6	0	0.744860	1.805774	-0.000024
5	6	0	-0.978394	0.381057	-0.000007
6	6	0	-2.243779	-1.421087	0.000013
7	7	0	-0.566112	1.677276	-0.000003
8	7	0	1.633399	0.774938	-0.000046
9	7	0	2.265321	-1.386904	-0.000088
10	7	0	-2.297706	-0.046561	-0.000027
11	7	0	-1.017310	-1.902121	-0.000007
12	6	0	-0.200193	-0.782507	-0.000022
13	1	0	-3.149287	-2.017160	0.000006
14	1	0	1.192950	2.794917	-0.000014
15	1	0	4.350875	-0.920287	-0.000100
16	6	0	-3.468119	0.801739	0.000268
17	1	0	-3.480546	1.444546	0.887973
18	1	0	-3.480285	1.445432	-0.886790
19	1	0	-4.362258	0.170951	-0.000180

9-Methyl-1,N^6-ethenoadenine: N9CH3 N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -583.113815462
Zero-point correction= 0.162595
(Hartree/Particle)
Thermal correction to Energy= 0.172515
Thermal correction to Enthalpy= 0.173459
Thermal correction to Gibbs Free Energy= 0.126585
Sum of electronic and zero-point Energies= -582.951221
Sum of electronic and thermal Energies= -582.941301
Sum of electronic and thermal Enthalpies= -582.940357
Sum of electronic and thermal Free Energies= -582.987231

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	108.254	38.887	98.654

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.276265	-0.614059	-0.294425
2	6	0	3.036425	0.670186	0.024077
3	6	0	1.135370	-0.703948	0.083491
4	6	0	0.680809	1.862186	-0.055425
5	6	0	-1.029834	0.371771	0.040141
6	6	0	-2.317689	-1.391750	0.047277
7	7	0	-0.565342	1.649802	-0.143723
8	7	0	1.608612	0.747848	0.389818
9	7	0	2.128027	-1.431139	-0.247164
10	7	0	-2.338088	-0.021504	-0.034783
11	7	0	-1.100103	-1.899271	0.144723
12	6	0	-0.284931	-0.810560	0.156887
13	1	0	-3.229890	-1.974171	0.038504
14	1	0	1.159751	2.825066	-0.196836
15	1	0	3.666529	1.543460	0.108806
16	1	0	4.227329	-1.047217	-0.576036

17	6	0	-3.515107	0.844613	-0.163380
18	1	0	-3.690356	1.380729	0.772706
19	1	0	-3.355332	1.559329	-0.972800
20	1	0	-4.377780	0.218680	-0.394325
21	1	0	1.580163	0.803338	1.426021

9-Methyl-1,N^6-ethenoadenine: N9CH3 N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -583.186516907
 Zero-point correction=                           0.164545
(Hartree/Particle)
 Thermal correction to Energy=                    0.174223
 Thermal correction to Enthalpy=                  0.175167
 Thermal correction to Gibbs Free Energy=         0.129368
 Sum of electronic and zero-point Energies=           -583.021972
 Sum of electronic and thermal Energies=              -583.012294
 Sum of electronic and thermal Enthalpies=            -583.011350
 Sum of electronic and thermal Free Energies=         -583.057149
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.327	38.442	96.392

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.317197	-0.637565	-0.000109
2	6	0	3.012746	0.698387	-0.000116
3	6	0	1.174293	-0.635822	-0.000040
4	6	0	0.801493	1.815721	-0.000045
5	6	0	-1.039170	0.353057	0.000030
6	6	0	-2.255978	-1.447366	-0.000013
7	7	0	-0.524280	1.626966	0.000002
8	7	0	1.619728	0.760614	-0.000064
9	7	0	2.193127	-1.439389	-0.000049
10	7	0	-2.340640	-0.065725	0.000049
11	7	0	-1.025929	-1.907319	0.000061
12	6	0	-0.235725	-0.792476	0.000010
13	1	0	-3.150614	-2.057222	-0.000013
14	1	0	1.194385	2.824895	-0.000061
15	1	0	3.626863	1.586576	-0.000148
16	1	0	4.305912	-1.076684	-0.000135
17	6	0	-3.555755	0.750286	0.000218
18	1	0	-3.601193	1.372192	0.899742
19	1	0	-3.600987	1.372824	-0.898878
20	1	0	-4.416449	0.080053	-0.000136
21	1	0	-1.126579	2.446013	0.000026

9-Methyl-1,N^6-ethenoadenine: N9CH3 N7 protonated

B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -583.217112157
 Zero-point correction=                           0.165609
(Hartree/Particle)
 Thermal correction to Energy=                    0.175126
 Thermal correction to Enthalpy=                  0.176070
 Thermal correction to Gibbs Free Energy=         0.130440
 Sum of electronic and zero-point Energies=           -583.051503
 Sum of electronic and thermal Energies=              -583.041986
 Sum of electronic and thermal Enthalpies=            -583.041042
 Sum of electronic and thermal Free Energies=         -583.086672

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 109.893             37.820             96.037
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.327179   -0.599311   -0.000146
    2          6             0        2.995234    0.735874   -0.000075
    3          6             0        1.196554   -0.582422   -0.000070
    4          6             0        0.725738    1.835982    0.000032
    5          6             0       -0.998273    0.407210    0.000049
    6          6             0       -2.331471   -1.355103    0.000024
    7          7             0       -0.571380    1.687975    0.000078
    8          7             0        1.608732    0.778162   -0.000036
    9          7             0        2.212137   -1.408435   -0.000149
   10          7             0       -2.325243   -0.018343    0.000069
   11          7             0       -1.065018   -1.811711   -0.000029
   12          6             0       -0.206969   -0.732429   -0.000022
   13          1             0       -3.215299   -1.976191    0.000020
   14          1             0        1.157223    2.831969    0.000056
   15          1             0        3.596335    1.632999   -0.000055
   16          1             0        4.321059   -1.025444   -0.000196
   17          6             0       -3.498315    0.869830    0.000212
   18          1             0       -3.469431    1.497891    0.892455
   19          1             0       -3.469098    1.498580   -0.891531
   20          1             0       -4.401125    0.258601   -0.000199
   21          1             0       -0.792339   -2.789729   -0.000108
 ---------------------------------------------------------------------
```

9-Methyl-1,N^6-ethenoadenine: N9CH3 N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -583.143962799
 Zero-point correction=                           0.164430
(Hartree/Particle)
 Thermal correction to Energy=                    0.173808
 Thermal correction to Enthalpy=                  0.174752
 Thermal correction to Gibbs Free Energy=         0.129725
 Sum of electronic and zero-point Energies=           -582.979533
 Sum of electronic and thermal Energies=              -582.970155
 Sum of electronic and thermal Enthalpies=            -582.969211
```

```
 Sum of electronic and thermal Free Energies=         -583.014238

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 109.066             37.869             94.768
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        3.273581   -0.702188    0.201463
    2          6             0        3.001090    0.646027    0.091994
    3          6             0        1.151331   -0.619671    0.021438
    4          6             0        0.803575    1.824436   -0.163369
    5          6             0       -0.951601    0.456689   -0.223122
    6          6             0       -2.292478   -1.419387   -0.220692
    7          7             0       -0.502717    1.711553   -0.264309
    8          7             0        1.629524    0.741178   -0.027065
    9          7             0        2.136851   -1.468895    0.157189
   10          7             0       -2.383772    0.094579   -0.315230
   11          7             0       -1.104648   -1.842173   -0.091278
   12          6             0       -0.252259   -0.717668   -0.090134
   13          1             0       -3.212450   -1.991482   -0.259174
   14          1             0        1.265244    2.806033   -0.187173
   15          1             0        3.641578    1.515682    0.088331
   16          1             0        4.247077   -1.161148    0.310940
   17          6             0       -3.270648    0.731450    0.740809
   18          1             0       -2.917181    0.402531    1.718354
   19          1             0       -3.175038    1.813061    0.639090
   20          1             0       -4.298905    0.410283    0.567275
   21          1             0       -2.752531    0.353214   -1.243112
 -------------------------------------------------------------------
```

9-Methyl-1,N^6-ethenoadenine: N9CH3 N10 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -583.228275471
 Zero-point correction=                           0.165572
(Hartree/Particle)
 Thermal correction to Energy=                    0.175188
 Thermal correction to Enthalpy=                  0.176132
 Thermal correction to Gibbs Free Energy=         0.129690
 Sum of electronic and zero-point Energies=           -583.062704
 Sum of electronic and thermal Energies=              -583.053088
 Sum of electronic and thermal Enthalpies=            -583.052144
 Sum of electronic and thermal Free Energies=         -583.098585

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 109.932             37.844             97.745

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        3.349384   -0.511515   -0.000105
```

2	6	0	2.950477	0.784976	-0.000082
3	6	0	1.114064	-0.532748	-0.000040
4	6	0	0.655804	1.846074	-0.000027
5	6	0	-1.062874	0.402781	0.000025
6	6	0	-2.266253	-1.426671	0.000050
7	7	0	-0.634708	1.682359	0.000012
8	7	0	1.546801	0.780208	-0.000051
9	7	0	2.214759	-1.312082	-0.000081
10	7	0	-2.354209	-0.052367	0.000039
11	7	0	-1.030405	-1.890609	0.000019
12	6	0	-0.265390	-0.758895	0.000004
13	1	0	-3.154448	-2.045777	0.000058
14	1	0	1.096218	2.837244	-0.000037
15	1	0	3.518287	1.702546	-0.000093
16	1	0	4.342932	-0.934007	-0.000137
17	6	0	-3.570367	0.766333	0.000189
18	1	0	-3.593330	1.395185	0.892991
19	1	0	-3.593007	1.395950	-0.892079
20	1	0	-4.433786	0.099883	-0.000259
21	1	0	2.192398	-2.325592	-0.000087

7-Methyl-1,N^6-ethenoadenine: NEUTRAL N7CH3
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -582.843186685 A.U.
Zero-point correction= 0.152031
(Hartree/Particle)
Thermal correction to Energy= 0.161448
Thermal correction to Enthalpy= 0.162392
Thermal correction to Gibbs Free Energy= 0.116666
Sum of electronic and zero-point Energies= -582.691155
Sum of electronic and thermal Energies= -582.681739
Sum of electronic and thermal Enthalpies= -582.680794
Sum of electronic and thermal Free Energies= -582.726520

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.310	36.764	96.238

Center Numer	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.712583	1.368509	-0.000014
2	6	0	-2.922125	0.009582	0.000018
3	6	0	-0.749366	0.519526	-0.000010
4	6	0	-1.246275	-1.884588	0.000014
5	6	0	0.926174	-1.251815	0.000013
6	6	0	2.767795	-0.190422	-0.000031
7	7	0	-0.003006	-2.254509	0.000022
8	7	0	-1.654659	-0.559637	0.000000
9	7	0	-1.374499	1.687080	-0.000044
10	7	0	2.290436	-1.416284	-0.000009

11	7	0	1.798291	0.787975	-0.000050
12	6	0	0.602287	0.113408	-0.000010
13	1	0	3.818938	0.069460	-0.000061
14	1	0	-3.466793	2.144465	-0.000017
15	1	0	-3.818601	-0.591944	0.000035
16	1	0	-2.042021	-2.623904	0.000035
17	6	0	1.994881	2.232349	0.000068
18	1	0	3.068544	2.434144	-0.000337
19	1	0	1.539989	2.677956	0.888824
20	1	0	1.539267	2.678166	-0.888200

7-Methyl-1,N^6-ethenoadenine: N7CH3 C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -582.237018314 A.U.
Zero-point correction= 0.136993
(Hartree/Particle)
Thermal correction to Energy= 0.146357
Thermal correction to Enthalpy= 0.147301
Thermal correction to Gibbs Free Energy= 0.102184
Sum of electronic and zero-point Energies= -582.100025
Sum of electronic and thermal Energies= -582.090662
Sum of electronic and thermal Enthalpies= -582.089717
Sum of electronic and thermal Free Energies= -582.134835

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.840	36.913	94.957

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.693048	1.355466	0.000017
2	6	0	-2.898384	-0.006610	0.000017
3	6	0	-0.713126	0.515021	0.000004
4	6	0	-1.205653	-1.883907	-0.000005
5	6	0	0.982338	-1.245003	-0.000014
6	6	0	2.909829	-0.160573	-0.000033
7	7	0	0.045514	-2.245815	-0.000015
8	7	0	-1.621411	-0.566679	0.000005
9	7	0	-1.365253	1.689486	0.000009
10	7	0	2.336403	-1.395659	-0.000028
11	7	0	1.842011	0.782228	-0.000020
12	6	0	0.637467	0.130801	-0.000004
13	1	0	-3.457348	2.124570	0.000024
14	1	0	-3.789923	-0.616497	0.000023
15	6	0	2.031784	2.215815	0.000039
16	1	0	3.112141	2.386611	-0.000193
17	1	0	1.583300	2.681070	0.887535
18	1	0	1.582874	2.681188	-0.887174
19	1	0	-1.999128	-2.627921	-0.000003

7-Methyl-1,N^6-ethenoadenine: N7CH3 C2 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.236222001     A.U.
   Zero-point correction=                           0.137031
(Hartree/Particle)
 Thermal correction to Energy=                    0.146622
 Thermal correction to Enthalpy=                  0.147566
 Thermal correction to Gibbs Free Energy=         0.101106
 Sum of electronic and zero-point Energies=           -582.099191
 Sum of electronic and thermal Energies=              -582.089600
 Sum of electronic and thermal Enthalpies=            -582.088656
 Sum of electronic and thermal Free Energies=         -582.135116

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  92.007             36.930             97.784

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.755966    1.295443   -0.000007
    2          6             0       -2.912073   -0.072937    0.000012
    3          6             0       -0.779385    0.483458   -0.000004
    4          6             0       -1.310856   -2.036372    0.000015
    5          6             0        0.903988   -1.257367   -0.000001
    6          6             0        2.754339   -0.163292   -0.000035
    7          7             0       -0.000184   -2.283722    0.000009
    8          7             0       -1.640144   -0.613749    0.000007
    9          7             0       -1.422920    1.656039   -0.000020
   10          7             0        2.289471   -1.394796   -0.000021
   11          7             0        1.773349    0.801644   -0.000037
   12          6             0        0.579670    0.103701   -0.000004
   13          1             0        3.802958    0.113500   -0.000053
   14          1             0       -3.533107    2.051578   -0.000011
   15          1             0       -3.777951   -0.718156    0.000028
   16          6             0        1.943505    2.240164    0.000062
   17          1             0        3.015099    2.466258   -0.000306
   18          1             0        1.478655    2.685980    0.886045
   19          1             0        1.478002    2.686142   -0.885491
 -------------------------------------------------------------------
```

7-Methyl-1,N^6-ethenoadenine: N7CH3 C11 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.213024964     A.U.
  Zero-point correction=                           0.136971
(Hartree/Particle)
 Thermal correction to Energy=                    0.145707
 Thermal correction to Enthalpy=                  0.146651
 Thermal correction to Gibbs Free Energy=         0.102812
 Sum of electronic and zero-point Energies=           -582.076054
```

```
 Sum of electronic and thermal Energies=             -582.067318
 Sum of electronic and thermal Enthalpies=           -582.066374
 Sum of electronic and thermal Free Energies=        -582.110213

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.432             34.983             92.266

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -2.791897    1.523327   -0.000041
    2          6             0       -2.950061    0.136997   -0.000016
    3          6             0       -0.771096    0.563002   -0.000006
    4          6             0       -1.314920   -1.824454    0.000013
    5          6             0        0.872819   -1.264922    0.000012
    6          6             0        2.738874   -0.226101   -0.000021
    7          7             0       -0.075110   -2.252098    0.000018
    8          7             0       -1.701662   -0.509605    0.000002
    9          7             0       -1.367046    1.735924   -0.000033
   10          7             0        2.243936   -1.446955   -0.000005
   11          7             0        1.778256    0.761572   -0.000026
   12          6             0        0.566492    0.104102    0.000005
   13          1             0       -3.849516   -0.468899   -0.000010
   14          6             0        1.975749    2.200076    0.000067
   15          1             0        3.051333    2.404479   -0.000465
   16          1             0        1.512964    2.649222    0.883887
   17          1             0        1.512029    2.649414   -0.883157
   18          1             0       -2.124604   -2.551330    0.000018
   19          1             0        3.793421    0.023088   -0.000040
 -------------------------------------------------------------------
```

7-Methyl-1,N^6-ethenoadenine: N7CH3 C12 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -582.240089349     A.U.
  Zero-point correction=                           0.138037
(Hartree/Particle)
 Thermal correction to Energy=                     0.146609
 Thermal correction to Enthalpy=                   0.147553
 Thermal correction to Gibbs Free Energy=          0.103992
 Sum of electronic and zero-point Energies=           -582.102053
 Sum of electronic and thermal Energies=              -582.093480
 Sum of electronic and thermal Enthalpies=            -582.092536
 Sum of electronic and thermal Free Energies=         -582.136098

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.999             34.308             91.683

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
```

1	6	0	-2.769883	1.300246	-0.000017
2	6	0	-3.037086	-0.072464	-0.000012
3	6	0	-0.784071	0.524722	-0.000005
4	6	0	-1.279787	-1.864275	0.000010
5	6	0	0.898120	-1.248027	0.000003
6	6	0	2.747859	-0.177415	-0.000019
7	7	0	-0.032239	-2.256777	0.000010
8	7	0	-1.709663	-0.558299	0.000002
9	7	0	-1.421343	1.677458	-0.000015
10	7	0	2.271470	-1.405392	-0.000011
11	7	0	1.767587	0.793472	-0.000031
12	6	0	0.566283	0.113726	-0.000003
13	6	0	1.942749	2.232610	0.000063
14	1	0	3.014738	2.454865	-0.000380
15	1	0	1.476209	2.676859	0.885272
16	1	0	1.475428	2.677027	-0.884642
17	1	0	-2.082878	-2.596003	0.000011
18	1	0	3.797675	0.090765	-0.000034
19	1	0	-3.516961	2.088505	-0.000026

7-Methyl-1,N^6-ethenoadenine: N7CH3 N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -583.206062655 A.U.
Zero-point correction= 0.165317
(Hartree/Particle)
Thermal correction to Energy= 0.174895
Thermal correction to Enthalpy= 0.175839
Thermal correction to Gibbs Free Energy= 0.130007
Sum of electronic and zero-point Energies= -583.040746
Sum of electronic and thermal Energies= -583.031168
Sum of electronic and thermal Enthalpies= -583.030224
Sum of electronic and thermal Free Energies= -583.076056

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.748	37.947	96.462

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.701318	1.419899	0.000004
2	6	0	-2.942029	0.071143	0.000000
3	6	0	-0.736331	0.566686	0.000002
4	6	0	-1.336966	-1.829397	-0.000003
5	6	0	0.940991	-1.206857	-0.000001
6	6	0	2.774431	-0.190383	-0.000017
7	7	0	-0.049749	-2.165470	-0.000004
8	7	0	-1.683166	-0.532398	0.000000
9	7	0	-1.352014	1.715540	0.000000
10	7	0	2.274031	-1.416822	-0.000011
11	7	0	1.821208	0.798150	-0.000017
12	6	0	0.611452	0.151905	0.000000

13	1	0	3.831081	0.042914	-0.000028
14	1	0	-3.439447	2.210548	0.000005
15	1	0	-3.854125	-0.506769	0.000002
16	1	0	-2.096587	-2.601291	-0.000006
17	6	0	2.046978	2.249626	0.000034
18	1	0	3.123310	2.426262	-0.000352
19	1	0	1.601018	2.693927	0.892321
20	1	0	1.600360	2.694077	-0.891845
21	1	0	0.218977	-3.148400	-0.000008

7-Methyl-1,N^6-ethenoadenine: N7CH3 N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -583.216892390     A.U.
  Zero-point correction=                           0.165550
(Hartree/Particle)
 Thermal correction to Energy=                    0.175058
 Thermal correction to Enthalpy=                  0.176002
 Thermal correction to Gibbs Free Energy=         0.130412
 Sum of electronic and zero-point Energies=           -583.051343
 Sum of electronic and thermal Energies=              -583.041835
 Sum of electronic and thermal Enthalpies=            -583.040890
 Sum of electronic and thermal Free Energies=         -583.086481

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 109.850             37.834             95.953
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.756000	1.336731	0.000004
2	6	0	-2.947105	-0.024995	-0.000002
3	6	0	-0.784093	0.523537	0.000004
4	6	0	-1.255859	-1.894713	0.000002
5	6	0	0.875538	-1.218101	-0.000004
6	6	0	2.770315	-0.061578	-0.000024
7	7	0	0.001360	-2.245253	-0.000004
8	7	0	-1.676491	-0.582379	0.000005
9	7	0	-1.418850	1.670065	0.000010
10	7	0	2.259215	-1.303275	-0.000019
11	7	0	1.773204	0.833991	-0.000015
12	6	0	0.575789	0.137490	0.000000
13	1	0	3.822930	0.181062	-0.000037
14	1	0	-3.518519	2.103514	0.000004
15	1	0	-3.839641	-0.632835	-0.000007
16	1	0	-2.030004	-2.655503	-0.000001
17	6	0	1.914766	2.301044	0.000036
18	1	0	2.976762	2.548686	-0.000331
19	1	0	1.432095	2.706056	0.891217
20	1	0	1.431458	2.706162	-0.890750
21	1	0	2.795746	-2.165677	-0.000036

7-Methyl-1,N^6-ethenoadenine: N7CH3 N10 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -583.211252648     A.U.
  Zero-point correction=                           0.165131
(Hartree/Particle)
 Thermal correction to Energy=                    0.174685
 Thermal correction to Enthalpy=                  0.175629
 Thermal correction to Gibbs Free Energy=         0.130172
 Sum of electronic and zero-point Energies=           -583.046124
 Sum of electronic and thermal Energies=              -583.036570
 Sum of electronic and thermal Enthalpies=            -583.035625
 Sum of electronic and thermal Free Energies=         -583.081083

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 109.617             38.143             95.673

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0       -2.810246    1.291176    0.000007
    2          6             0       -2.925948   -0.058529    0.000007
    3          6             0       -0.723637    0.463881   -0.000005
    4          6             0       -1.212399   -1.912238   -0.000002
    5          6             0        0.953612   -1.262066    0.000000
    6          6             0        2.787189   -0.201340   -0.000015
    7          7             0        0.033488   -2.260083    0.000001
    8          7             0       -1.626620   -0.582625   -0.000002
    9          7             0       -1.455896    1.606394    0.000000
   10          7             0        2.304706   -1.424870   -0.000005
   11          7             0        1.829367    0.788571   -0.000030
   12          6             0        0.627301    0.118926   -0.000008
   13          1             0        3.841286    0.048172   -0.000026
   14          1             0       -3.570964    2.057169    0.000014
   15          1             0       -3.796271   -0.696680    0.000012
   16          1             0       -2.006774   -2.651869    0.000001
   17          6             0        2.067081    2.230924    0.000038
   18          1             0        3.144886    2.402465   -0.000279
   19          1             0        1.646553    2.689872    0.900372
   20          1             0        1.646029    2.690025   -0.899972
   21          1             0       -1.077777    2.544739    0.000001
 -----------------------------------------------------------------------
```

Guanine: NEUTRAL 7H-keto-guanine
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.566882870     A.U.
 Zero-point correction=                           0.116615
(Hartree/Particle)
 Thermal correction to Energy=                    0.125007
```

```
 Thermal correction to Enthalpy=                  0.125951
 Thermal correction to Gibbs Free Energy=         0.083366
 Sum of electronic and zero-point Energies=           -542.450268
 Sum of electronic and thermal Energies=              -542.441876
 Sum of electronic and thermal Enthalpies=            -542.440932
 Sum of electronic and thermal Free Energies=         -542.483517

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  78.443             33.000             89.628
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.806105    0.442288    0.016450
    2          6             0       -0.539167   -0.908378    0.005173
    3          6             0        1.748647   -0.361731    0.000294
    4          6             0        0.231771    1.458127    0.000474
    5          6             0       -2.647030   -0.769712   -0.003936
    6          1             0       -3.701465   -1.009071   -0.010871
    7          7             0        1.528006    0.924575    0.016925
    8          7             0        0.772545   -1.338197    0.006971
    9          7             0       -1.667083   -1.669148   -0.006800
   10          7             0       -2.185752    0.510765    0.010852
   11          1             0       -2.726683    1.365901    0.014770
   12          7             0        3.048375   -0.824446   -0.073508
   13          1             0        3.728157   -0.085923    0.066686
   14          1             0        3.270955   -1.679826    0.422182
   15          8             0        0.005045    2.666640   -0.015017
   16          1             0        0.987349   -2.312607   -0.164442
 ---------------------------------------------------------------------
```

Guanine: 7H-keto-guanine N1 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.033154451     A.U.
 Zero-point correction=                           0.103458
(Hartree/Particle)
 Thermal correction to Energy=                    0.111428
 Thermal correction to Enthalpy=                  0.112372
 Thermal correction to Gibbs Free Energy=         0.070617
 Sum of electronic and zero-point Energies=           -541.929697
 Sum of electronic and thermal Energies=              -541.921727
 Sum of electronic and thermal Enthalpies=            -541.920783
 Sum of electronic and thermal Free Energies=         -541.962537

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.922             31.355             87.880

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.767461    0.420521   -0.011070
```

2	6	0	-0.478974	-0.941976	-0.006030
3	6	0	1.695127	-0.436264	-0.017228
4	6	0	0.261187	1.430005	-0.003268
5	6	0	-2.618511	-0.774188	0.010449
6	1	0	-3.679298	-0.995858	0.018235
7	7	0	1.531835	0.899203	-0.007642
8	7	0	0.789506	-1.424955	-0.008260
9	7	0	-1.657041	-1.681960	0.006858
10	7	0	-2.148591	0.509522	0.000295
11	1	0	-2.672704	1.372785	0.002548
12	7	0	3.039845	-0.860070	-0.075560
13	1	0	3.668961	-0.166589	0.312764
14	1	0	3.165494	-1.784122	0.322542
15	8	0	0.010057	2.661626	0.012119

Guanine: 7H-keto-guanine N2Ha deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.012711053 A.U.
Zero-point correction= 0.102112
(Hartree/Particle)
Thermal correction to Energy= 0.110337
Thermal correction to Enthalpy= 0.111281
Thermal correction to Gibbs Free Energy= 0.068820
Sum of electronic and zero-point Energies= -541.910599
Sum of electronic and thermal Energies= -541.902375
Sum of electronic and thermal Enthalpies= -541.901430
Sum of electronic and thermal Free Energies= -541.943891

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.237	31.819	89.366

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.755031	0.450962	0.000673
2	6	0	-0.495151	-0.934520	0.000129
3	6	0	1.778108	-0.670176	-0.000053
4	6	0	0.288875	1.404770	0.000004
5	6	0	-2.641526	-0.676551	-0.000095
6	1	0	-3.710067	-0.860879	-0.000389
7	7	0	1.521220	0.748696	-0.000768
8	1	0	2.322225	1.368967	-0.000352
9	7	0	0.707933	-1.513525	0.000072
10	7	0	-1.719412	-1.617991	-0.000358
11	7	0	-2.139130	0.591797	0.000006
12	1	0	-2.645905	1.464298	0.001240
13	7	0	3.012314	-1.113132	0.000354
14	1	0	3.666563	-0.325287	0.000345
15	8	0	0.204382	2.654385	0.000008

Guanine: 7H-keto-guanine N2Hb deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.024223288     A.U.
 Zero-point correction=                           0.102871
(Hartree/Particle)
 Thermal correction to Energy=                    0.110961
 Thermal correction to Enthalpy=                  0.111905
 Thermal correction to Gibbs Free Energy=         0.069716
 Sum of electronic and zero-point Energies=           -541.921352
 Sum of electronic and thermal Energies=              -541.913262
 Sum of electronic and thermal Enthalpies=            -541.912318
 Sum of electronic and thermal Free Energies=         -541.954507

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.629             31.384             88.794
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.755661	0.438857	0.000138
2	6	0	-0.475186	-0.939478	0.000056
3	6	0	1.788979	-0.604996	0.000141
4	6	0	0.272349	1.418233	-0.000481
5	6	0	-2.624021	-0.718615	-0.000062
6	1	0	-3.689211	-0.920526	-0.000110
7	7	0	1.512534	0.793465	-0.000303
8	1	0	2.328591	1.393453	0.000436
9	7	0	0.747060	-1.490035	0.000213
10	7	0	-1.684440	-1.645004	-0.000008
11	7	0	-2.140676	0.556499	-0.000140
12	1	0	-2.659501	1.422073	0.000592
13	7	0	3.063381	-0.906501	0.000005
14	1	0	3.128010	-1.926036	-0.000425
15	8	0	0.146042	2.663507	0.000296

Guanine: 7H-keto-guanine N7 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.032671794     A.U.
 Zero-point correction=                           0.103540
(Hartree/Particle)
 Thermal correction to Energy=                    0.111519
 Thermal correction to Enthalpy=                  0.112463
 Thermal correction to Gibbs Free Energy=         0.070626
 Sum of electronic and zero-point Energies=           -541.929132
 Sum of electronic and thermal Energies=              -541.921153
 Sum of electronic and thermal Enthalpies=            -541.920209
 Sum of electronic and thermal Free Energies=         -541.962046
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.979	31.121	88.054

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.894946	0.466650	0.015912
2	6	0	-0.575214	-0.921753	-0.006245
3	6	0	1.644852	-0.547593	-0.011071
4	6	0	0.139053	1.449350	0.002889
5	6	0	-2.670134	-0.670502	0.004428
6	1	0	-3.726649	-0.927631	0.004330
7	7	0	1.424421	0.810444	-0.005088
8	1	0	2.202171	1.446457	-0.136827
9	7	0	0.708574	-1.442547	0.000330
10	7	0	-1.715290	-1.645048	-0.010755
11	7	0	-2.263575	0.605591	0.020864
12	7	0	3.007052	-0.932789	-0.074089
13	1	0	3.568293	-0.512778	0.664799
14	1	0	3.052742	-1.945542	0.002345
15	8	0	0.114187	2.689127	-0.011120

Guanine: 7H-keto-guanine C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.970546070 A.U.
Zero-point correction= 0.102623
(Hartree/Particle)
Thermal correction to Energy= 0.110917
Thermal correction to Enthalpy= 0.111861
Thermal correction to Gibbs Free Energy= 0.069496
Sum of electronic and zero-point Energies= -541.867923
Sum of electronic and thermal Energies= -541.859629
Sum of electronic and thermal Enthalpies= -541.858685
Sum of electronic and thermal Free Energies= -541.901050

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.602	32.388	89.166

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.875944	0.419957	0.016738
2	6	0	-0.559347	-0.955460	-0.004871
3	6	0	1.658209	-0.504005	-0.009979
4	6	0	0.101169	1.434065	0.002672
5	6	0	-2.776178	-0.871748	0.001817
6	7	0	1.407464	0.848702	-0.003553
7	1	0	2.166402	1.505471	-0.142526
8	7	0	0.745074	-1.424751	0.001598

9	7	0	-1.679076	-1.712158	-0.010480
10	7	0	-2.259472	0.425746	0.017570
11	1	0	-2.830939	1.257248	0.026399
12	7	0	3.026035	-0.857237	-0.074947
13	1	0	3.586482	-0.414213	0.650140
14	1	0	3.098522	-1.867857	0.006583
15	8	0	0.001488	2.677547	-0.011272

Guanine: 7H-keto-guanine OHa protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.917287030 A.U.
Zero-point correction= 0.127655
(Hartree/Particle)
Thermal correction to Energy= 0.136944
Thermal correction to Enthalpy= 0.137888
Thermal correction to Gibbs Free Energy= 0.093471
Sum of electronic and zero-point Energies= -542.789632
Sum of electronic and thermal Energies= -542.780344
Sum of electronic and thermal Enthalpies= -542.779399
Sum of electronic and thermal Free Energies= -542.823817

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.933	35.605	93.484

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.827659	0.419580	0.000819
2	6	0	-0.518142	-0.975838	-0.002160
3	6	0	1.702438	-0.577496	0.002947
4	6	0	0.195767	1.330891	0.000159
5	6	0	-2.637928	-0.810022	0.000563
6	1	0	-3.693513	-1.052726	0.000223
7	7	0	1.463713	0.802084	-0.001758
8	1	0	2.257794	1.433740	-0.046355
9	7	0	0.730842	-1.462470	0.003936
10	7	0	-1.666191	-1.705194	-0.002289
11	7	0	-2.207120	0.486313	0.003965
12	1	0	-2.785912	1.317825	0.004929
13	7	0	2.987989	-0.979716	-0.020802
14	1	0	3.776770	-0.365836	0.126589
15	1	0	3.156417	-1.978046	0.020479
16	8	0	-0.018066	2.642266	-0.003270
17	1	0	0.781487	3.197101	0.024957

Guanine: 7H-keto-guanine OHb protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.919803797   A.U.
 Zero-point correction=   0.127987
(Hartree/Particle)
 Thermal correction to Energy=   0.137101
 Thermal correction to Enthalpy=   0.138045
 Thermal correction to Gibbs Free Energy=   0.094153
 Sum of electronic and zero-point Energies=   -542.791817
 Sum of electronic and thermal Energies=   -542.782703
 Sum of electronic and thermal Enthalpies=   -542.781759
 Sum of electronic and thermal Free Energies=   -542.825651

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.032	35.428	92.379

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.834757	0.436881	0.000019
2	6	0	0.524417	-0.964786	-0.000251
3	6	0	-1.698328	-0.582858	0.000180
4	6	0	-0.207993	1.330214	-0.000101
5	6	0	2.646353	-0.807080	0.000113
6	1	0	3.702034	-1.050286	0.000225
7	7	0	-1.464584	0.786165	-0.000237
8	1	0	-2.237771	1.447281	-0.001320
9	7	0	-0.714746	-1.462822	-0.000014
10	7	0	1.675295	-1.695417	-0.000279
11	7	0	2.220903	0.494649	0.000346
12	1	0	2.826280	1.305853	0.001155
13	7	0	-2.975012	-1.001089	-0.000289
14	1	0	-3.776036	-0.385507	0.003905
15	1	0	-3.139227	-2.000620	0.000176
16	8	0	-0.227467	2.661547	0.000195
17	1	0	0.656224	3.066274	-0.002139

Guanine: 7H-keto-guanine N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.941575945   A.U.
 Zero-point correction=   0.129468
(Hartree/Particle)
 Thermal correction to Energy=   0.138234
 Thermal correction to Enthalpy=   0.139178
 Thermal correction to Gibbs Free Energy=   0.095975
 Sum of electronic and zero-point Energies=   -542.812108
 Sum of electronic and thermal Energies=   -542.803342
 Sum of electronic and thermal Enthalpies=   -542.802398
 Sum of electronic and thermal Free Energies=   -542.845601

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.743	34.569	90.928

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.866042	0.460882	0.000091
2	6	0	-0.571450	-0.890047	-0.000135
3	6	0	1.758054	-0.459582	0.000026
4	6	0	0.138489	1.480285	-0.000068
5	6	0	-2.673920	-0.787964	0.000229
6	1	0	-3.722626	-1.052630	0.000427
7	7	0	1.461136	0.858201	-0.000034
8	1	0	2.217535	1.538519	0.000333
9	7	0	0.743751	-1.345228	-0.000534
10	7	0	-1.671325	-1.665245	-0.000201
11	7	0	-2.244239	0.501118	0.000284
12	1	0	-2.818846	1.337258	0.000607
13	7	0	3.030349	-0.876963	0.000362
14	1	0	3.803297	-0.223457	0.000586
15	1	0	3.269500	-1.860792	0.000547
16	8	0	0.048893	2.685456	-0.000266
17	1	0	0.911500	-2.347172	-0.000362

Guanine: 7H-keto-guanine N9 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.950055488     A.U.
 Zero-point correction=                           0.130034
(Hartree/Particle)
 Thermal correction to Energy=                    0.138563
 Thermal correction to Enthalpy=                  0.139508
 Thermal correction to Gibbs Free Energy=         0.096742
 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=         -542.853314

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.950             33.893             90.008
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.788737	0.476061	-0.000116
2	6	0	0.472545	-0.872842	-0.000073
3	6	0	-1.729137	-0.543392	-0.000003
4	6	0	-0.250820	1.472821	-0.000040
5	6	0	2.696552	-0.643249	0.000062
6	1	0	3.751026	-0.877762	0.000090
7	7	0	-1.515690	0.820516	0.000086
8	1	0	-2.305529	1.461405	0.000311
9	7	0	-0.739067	-1.432932	-0.000086

10	7	0	1.691940	-1.542387	0.000087
11	7	0	2.168714	0.579080	-0.000088
12	1	0	2.693518	1.449787	-0.000254
13	7	0	-2.996840	-0.984787	0.000019
14	1	0	-3.800924	-0.373049	-0.000323
15	1	0	-3.155941	-1.984305	0.000018
16	8	0	-0.139740	2.682863	0.000077
17	1	0	1.805109	-2.551811	0.000444

Guanine: 7H-keto-guanine N2 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.895334433 A.U.
Zero-point correction= 0.130508
(Hartree/Particle)
Thermal correction to Energy= 0.139019
Thermal correction to Enthalpy= 0.139963
Thermal correction to Gibbs Free Energy= 0.097037
Sum of electronic and zero-point Energies= -542.764826
Sum of electronic and thermal Energies= -542.756316
Sum of electronic and thermal Enthalpies= -542.755372
Sum of electronic and thermal Free Energies= -542.798297

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.236	33.031	90.345

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.888459	0.420892	0.000849
2	6	0	0.539820	-0.933813	0.000100
3	6	0	-1.624664	-0.419058	-0.000202
4	6	0	-0.066657	1.492062	0.000064
5	6	0	2.655545	-0.879539	-0.000296
6	1	0	3.700137	-1.161258	-0.000560
7	7	0	-1.405170	0.922844	0.000343
8	1	0	-2.148670	1.617367	-0.001648
9	7	0	-0.769991	-1.368476	-0.000087
10	7	0	1.641022	-1.728092	-0.000507
11	7	0	2.257323	0.430044	0.000433
12	1	0	2.852822	1.251361	0.001112
13	7	0	-3.050009	-0.871361	0.000112
14	1	0	-3.574618	-0.568776	-0.834272
15	1	0	-3.012067	-1.903649	-0.001145
16	8	0	0.086050	2.694730	-0.000594
17	1	0	-3.573248	-0.570854	0.836125

Guanine: NEUTRAL 9H-keto-guanine
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.576444281   A.U.
 Zero-point correction=   0.116755
(Hartree/Particle)
 Thermal correction to Energy=   0.124994
 Thermal correction to Enthalpy=   0.125939
 Thermal correction to Gibbs Free Energy=   0.083742
 Sum of electronic and zero-point Energies=   -542.459689
 Sum of electronic and thermal Energies=   -542.451450
 Sum of electronic and thermal Enthalpies=   -542.450506
 Sum of electronic and thermal Free Energies=   -542.492702

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.435	32.779	88.810

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856535	0.504040	0.008223
2	6	0	-0.528998	-0.853216	-0.000749
3	6	0	1.676161	-0.565196	-0.001781
4	6	0	0.210098	1.471320	0.003226
5	6	0	-2.717260	-0.532967	0.000892
6	1	0	-3.768784	-0.787557	-0.001056
7	7	0	1.477977	0.792460	-0.003104
8	1	0	2.271610	1.420671	-0.078410
9	7	0	0.696971	-1.438816	0.007685
10	7	0	-1.732922	-1.507762	-0.004167
11	7	0	-2.227332	0.680411	0.008192
12	7	0	2.980833	-1.005759	-0.068816
13	1	0	3.691005	-0.447275	0.388610
14	1	0	3.075579	-2.000638	0.097235
15	8	0	0.189915	2.692298	-0.003946
16	1	0	-1.858205	-2.511211	-0.012209

Guanine: 9H-keto-guanine N1 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.028432574   A.U.
 Zero-point correction=   0.103100
(Hartree/Particle)
 Thermal correction to Energy=   0.111150
 Thermal correction to Enthalpy=   0.112094
 Thermal correction to Gibbs Free Energy=   0.070169
 Sum of electronic and zero-point Energies=   -541.925333
 Sum of electronic and thermal Energies=   -541.917283
 Sum of electronic and thermal Enthalpies=   -541.916339
 Sum of electronic and thermal Free Energies=   -541.958263

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.748	31.630	88.238

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.807566	0.503378	-0.005319
2	6	0	-0.496921	-0.857862	-0.004496
3	6	0	1.676341	-0.477808	-0.017218
4	6	0	0.300051	1.454409	-0.002612
5	6	0	-2.693246	-0.523042	0.007262
6	1	0	-3.748592	-0.768801	0.012284
7	7	0	1.557714	0.846389	-0.007797
8	7	0	0.719822	-1.433662	-0.008985
9	7	0	-1.716342	-1.509150	0.004679
10	7	0	-2.187851	0.685808	0.003708
11	7	0	2.996319	-0.970688	-0.075624
12	1	0	3.660518	-0.294375	0.283471
13	1	0	3.087256	-1.886852	0.349198
14	8	0	0.173271	2.691913	0.009832
15	1	0	-1.844946	-2.510613	-0.001191

Guanine: 9H-keto-guanine N2Ha deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.020031757 A.U.
Zero-point correction= 0.102454
(Hartree/Particle)
Thermal correction to Energy= 0.110504
Thermal correction to Enthalpy= 0.111448
Thermal correction to Gibbs Free Energy= 0.069401
Sum of electronic and zero-point Energies= -541.917578
Sum of electronic and thermal Energies= -541.909528
Sum of electronic and thermal Enthalpies= -541.908584
Sum of electronic and thermal Free Energies= -541.950631

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.342	31.565	88.496

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.791767	0.530210	0.000208
2	6	0	0.510884	-0.852860	-0.000417
3	6	0	-1.749909	-0.713024	0.000095
4	6	0	-0.325849	1.426709	-0.000083
5	6	0	2.707502	-0.421106	0.000122
6	1	0	3.771005	-0.627193	-0.000352
7	7	0	-1.534807	0.700288	-0.001338
8	1	0	-2.355774	1.293946	-0.000963
9	7	0	-0.642282	-1.514338	-0.000660
10	7	0	1.764753	-1.443136	-0.000414
11	7	0	2.161934	0.767289	0.001063
12	7	0	-2.959234	-1.214710	0.001212

13	1	0	-3.649714	-0.458886	0.001589
14	8	0	-0.353870	2.668073	0.000076
15	1	0	1.926526	-2.439779	0.000520

Guanine: 9H-keto-guanine N2Hb deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.029279355 A.U.
Zero-point correction= 0.102989
(Hartree/Particle)
Thermal correction to Energy= 0.110968
Thermal correction to Enthalpy= 0.111912
Thermal correction to Gibbs Free Energy= 0.069996
Sum of electronic and zero-point Energies= -541.926290
Sum of electronic and thermal Energies= -541.918311
Sum of electronic and thermal Enthalpies= -541.917367
Sum of electronic and thermal Free Energies= -541.959283

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.634	31.281	88.220

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.793121	0.519004	0.000040
2	6	0	0.493857	-0.857623	0.000003
3	6	0	-1.763116	-0.652209	0.000042
4	6	0	-0.311943	1.440295	0.000037
5	6	0	2.695630	-0.460781	-0.000136
6	1	0	3.755768	-0.683016	-0.000360
7	7	0	-1.529463	0.743276	0.000333
8	1	0	-2.364175	1.317232	-0.000051
9	7	0	-0.678958	-1.493800	0.000060
10	7	0	1.736350	-1.468678	-0.000206
11	7	0	2.165831	0.734961	0.000183
12	7	0	-3.018729	-1.017038	-0.000174
13	1	0	-3.035778	-2.038675	-0.000369
14	8	0	-0.301368	2.681083	-0.000200
15	1	0	1.884619	-2.467364	0.001086

Guanine: 9H-keto-guanine C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.962954807 A.U.
Zero-point correction= 0.102331
(Hartree/Particle)
Thermal correction to Energy= 0.110629
Thermal correction to Enthalpy= 0.111574
Thermal correction to Gibbs Free Energy= 0.069210

```
 Sum of electronic and zero-point Energies=          -541.860624
 Sum of electronic and thermal Energies=             -541.852325
 Sum of electronic and thermal Enthalpies=           -541.851381
 Sum of electronic and thermal Free Energies=        -541.893745

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.421             32.524             89.162

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.922421    0.476453    0.012655
    2          6             0       -0.557163   -0.880371   -0.005786
    3          6             0        1.650298   -0.533499   -0.010180
    4          6             0        0.121056    1.455506    0.002094
    5          6             0       -2.853555   -0.630458    0.006625
    6          7             0        1.415629    0.814604   -0.009496
    7          1             0        2.188397    1.460490   -0.125019
    8          7             0        0.702344   -1.427591    0.002304
    9          7             0       -1.744861   -1.542381   -0.007522
   10          7             0       -2.300533    0.605110    0.018584
   11          7             0        3.004738   -0.928129   -0.073697
   12          1             0        3.583244   -0.487496    0.638500
   13          1             0        3.055503   -1.938634    0.020930
   14          8             0        0.105719    2.692013   -0.007599
   15          1             0       -1.843408   -2.547543   -0.017267
 ---------------------------------------------------------------------
```

Guanine: 9H-keto-guanine N9 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.032671263     A.U.
 Zero-point correction=                           0.103540
(Hartree/Particle)
 Thermal correction to Energy=                    0.111518
 Thermal correction to Enthalpy=                  0.112463
 Thermal correction to Gibbs Free Energy=         0.070627
 Sum of electronic and zero-point Energies=           -541.929132
 Sum of electronic and thermal Energies=              -541.921153
 Sum of electronic and thermal Enthalpies=            -541.920209
 Sum of electronic and thermal Free Energies=         -541.962045

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.979             31.120             88.050

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.895064    0.466739    0.015721
    2          6             0       -0.575357   -0.921632   -0.005731
```

3	6	0	1.644574	-0.547691	-0.010952
4	6	0	0.139305	1.449375	0.003185
5	6	0	-2.670119	-0.670103	0.004522
6	1	0	-3.726468	-0.927627	0.004342
7	7	0	1.424400	0.810304	-0.004548
8	1	0	2.202261	1.446292	-0.135914
9	7	0	0.708237	-1.442621	0.000319
10	7	0	-1.715409	-1.645193	-0.011427
11	7	0	-2.263411	0.605694	0.021227
12	7	0	3.007173	-0.933054	-0.074535
13	1	0	3.568794	-0.511510	0.663373
14	1	0	3.053139	-1.945704	0.004305
15	8	0	0.114414	2.689064	-0.011729

Guanine: 9H-keto-guanine N2Hb protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.938237486 A.U.
Zero-point correction= 0.129249
(Hartree/Particle)
Thermal correction to Energy= 0.137882
Thermal correction to Enthalpy= 0.138826
Thermal correction to Gibbs Free Energy= 0.095938
Sum of electronic and zero-point Energies= -542.808989
Sum of electronic and thermal Energies= -542.800355
Sum of electronic and thermal Enthalpies= -542.799411
Sum of electronic and thermal Free Energies= -542.842300

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.522	34.326	90.267

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.845775	0.442257	0.000005
2	6	0	-0.503630	-0.932286	0.000020
3	6	0	1.702865	-0.569011	0.000087
4	6	0	0.203795	1.336426	0.000106
5	6	0	-2.693452	-0.586751	-0.000034
6	1	0	-3.744531	-0.844880	-0.000056
7	7	0	1.463784	0.801070	0.000089
8	1	0	2.238375	1.460818	-0.000110
9	7	0	0.721838	-1.459201	0.000112
10	7	0	-1.705848	-1.570104	0.000009
11	7	0	-2.214539	0.627855	-0.000025
12	7	0	2.981482	-0.979531	-0.000441
13	1	0	3.776362	-0.355745	0.001184
14	1	0	3.158590	-1.976475	0.000403
15	8	0	0.159424	2.654195	-0.000055
16	1	0	-1.848747	-2.574430	-0.000113
17	1	0	-0.765274	2.972719	-0.000178

Guanine: 9H-keto-guanine N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.921133476     A.U.
 Zero-point correction=                           0.128412
(Hartree/Particle)
 Thermal correction to Energy=                    0.137488
 Thermal correction to Enthalpy=                  0.138432
 Thermal correction to Gibbs Free Energy=         0.094589
 Sum of electronic and zero-point Energies=           -542.792722
 Sum of electronic and thermal Energies=              -542.783646
 Sum of electronic and thermal Enthalpies=            -542.782702
 Sum of electronic and thermal Free Energies=         -542.826544

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.275             35.400             92.275
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891105	0.506228	-0.000105
2	6	0	-0.579559	-0.841091	-0.000173
3	6	0	1.752295	-0.482875	0.000043
4	6	0	0.158809	1.497911	-0.000256
5	6	0	-2.750571	-0.530716	0.000416
6	1	0	-3.800506	-0.790901	0.000975
7	7	0	1.481221	0.830235	0.000150
8	1	0	2.250305	1.496780	0.001176
9	7	0	0.712666	-1.352252	-0.001234
10	7	0	-1.761702	-1.512718	0.000089
11	7	0	-2.254823	0.676414	0.000563
12	7	0	3.011765	-0.940127	0.000363
13	1	0	3.801046	-0.305987	0.001354
14	1	0	3.228316	-1.928898	0.002634
15	8	0	0.135920	2.698304	-0.000409
16	1	0	-1.917415	-2.514375	-0.000714
17	1	0	0.887789	-2.350665	-0.001215

Guanine: 9H-keto-guanine N7 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.950055480     A.U.
 Zero-point correction=                           0.130035
(Hartree/Particle)
 Thermal correction to Energy=                    0.138564
 Thermal correction to Enthalpy=                  0.139508
 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

                    E (Thermal)             CV               S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.950             33.892            90.006
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.788713    0.476036   -0.000239
    2          6             0        0.472583   -0.872884   -0.000104
    3          6             0       -1.729115   -0.543431   -0.000038
    4          6             0       -0.250927    1.472786   -0.000026
    5          6             0        2.696544   -0.643211    0.000128
    6          1             0        3.751030   -0.877645    0.000197
    7          7             0       -1.515688    0.820541   -0.000017
    8          1             0       -2.305619    1.461326    0.000054
    9          7             0       -0.739038   -1.432947   -0.000054
   10          7             0        1.691991   -1.542391    0.000091
   11          7             0        2.168632    0.579144   -0.000045
   12          7             0       -2.996822   -0.984753   -0.000111
   13          1             0       -3.800928   -0.373031    0.000830
   14          1             0       -3.156022   -1.984259    0.000432
   15          8             0       -0.139672    2.682820    0.000138
   16          1             0        1.805259   -2.551804    0.000256
   17          1             0        2.693349    1.449916   -0.000246
 -------------------------------------------------------------------
```

Guanine: 9H-keto-guanine N2 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.888496527     A.U.
Zero-point correction=                           0.130159
(Hartree/Particle)
 Thermal correction to Energy=                    0.138731
 Thermal correction to Enthalpy=                  0.139675
 Thermal correction to Gibbs Free Energy=         0.096621
 Sum of electronic and zero-point Energies=           -542.758339
 Sum of electronic and thermal Energies=              -542.749766
 Sum of electronic and thermal Enthalpies=            -542.748822
 Sum of electronic and thermal Free Energies=         -542.791877

                    E (Thermal)             CV               S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.055             33.282            90.616

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.923490    0.477185    0.000197
    2          6             0        0.545684   -0.868539    0.000113
    3          6             0       -1.614657   -0.447421    0.000193
    4          6             0       -0.084684    1.517678    0.000340
```

5	6	0	2.730181	-0.640488	0.000732
6	1	0	3.772455	-0.930743	0.000830
7	7	0	-1.421900	0.889898	0.000114
8	1	0	-2.181616	1.567057	-0.000504
9	7	0	-0.726257	-1.375628	0.000191
10	7	0	1.715867	-1.573528	-0.000565
11	7	0	2.284782	0.597153	-0.000537
12	7	0	-3.025712	-0.936223	-0.000117
13	1	0	-3.556106	-0.640733	-0.834030
14	1	0	-2.975501	-1.967225	-0.001428
15	8	0	-0.013289	2.719347	-0.000226
16	1	0	1.815105	-2.582307	-0.001095
17	1	0	-3.555563	-0.643012	0.834977

Guanine: NEUTRAL 9H-trans-enol-guanine
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.576444281 A.U.
Zero-point correction= 0.116755
(Hartree/Particle)
Thermal correction to Energy= 0.124994
Thermal correction to Enthalpy= 0.125939
Thermal correction to Gibbs Free Energy= 0.083742
Sum of electronic and zero-point Energies= -542.459689
Sum of electronic and thermal Energies= -542.451450
Sum of electronic and thermal Enthalpies= -542.450506
Sum of electronic and thermal Free Energies= -542.492702

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.435	32.779	88.810

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856535	0.504040	0.008223
2	6	0	-0.528998	-0.853216	-0.000749
3	6	0	1.676161	-0.565196	-0.001781
4	6	0	0.210098	1.471320	0.003226
5	6	0	-2.717260	-0.532967	0.000892
6	1	0	-3.768784	-0.787557	-0.001056
7	7	0	1.477977	0.792460	-0.003104
8	1	0	2.271610	1.420671	-0.078410
9	7	0	0.696971	-1.438816	0.007685
10	7	0	-1.732922	-1.507762	-0.004167
11	7	0	-2.227332	0.680411	0.008192
12	7	0	2.980833	-1.005759	-0.068816
13	1	0	3.691005	-0.447275	0.388610
14	1	0	3.075579	-2.000638	0.097235
15	8	0	0.189915	2.692298	-0.003946
16	1	0	-1.858205	-2.511211	-0.012209

Guanine: 9H-trans-enol-guanine N2Ha deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.990238811     A.U.
 Zero-point correction=                           0.102147
(Hartree/Particle)
 Thermal correction to Energy=                    0.110299
 Thermal correction to Enthalpy=                  0.111243
 Thermal correction to Gibbs Free Energy=         0.068950
 Sum of electronic and zero-point Energies=           -541.888092
 Sum of electronic and thermal Energies=              -541.879940
 Sum of electronic and thermal Enthalpies=            -541.878996
 Sum of electronic and thermal Free Energies=         -541.921289

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.214             31.857             89.013


---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.745185    0.451669    0.001538
    2          6             0        0.452872   -0.926385    0.000062
    3          6             0       -1.800096   -0.626448   -0.000142
    4          6             0       -0.399456    1.277856   -0.000091
    5          6             0        2.659284   -0.494434   -0.000114
    6          1             0        3.722596   -0.698636   -0.000502
    7          7             0       -1.602297    0.786937   -0.001058
    8          7             0       -0.720649   -1.516880   -0.001072
    9          7             0        1.715583   -1.517368   -0.000720
   10          7             0        2.112150    0.699532    0.001308
   11          7             0       -3.016417   -1.106843    0.001224
   12          1             0       -3.648812   -0.302995    0.001827
   13          8             0       -0.253960    2.647885   -0.000647
   14          1             0        1.888447   -2.512013   -0.000725
   15          1             0        0.704113    2.819365   -0.000717
 ---------------------------------------------------------------------
```

Guanine: 9H-trans-enol-guanine N2Hb deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.989517260     A.U.
 Zero-point correction=                           0.102101
(Hartree/Particle)
 Thermal correction to Energy=                    0.110260
 Thermal correction to Enthalpy=                  0.111204
 Thermal correction to Gibbs Free Energy=         0.068888
 Sum of electronic and zero-point Energies=           -541.887416
 Sum of electronic and thermal Energies=              -541.879258
 Sum of electronic and thermal Enthalpies=            -541.878313
 Sum of electronic and thermal Free Energies=         -541.920629
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.189	31.864	89.060

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.756144	0.436263	0.000931
2	6	0	0.417770	-0.928719	-0.000107
3	6	0	-1.832852	-0.527332	-0.000042
4	6	0	-0.361867	1.303908	0.000040
5	6	0	2.637387	-0.575833	0.000160
6	1	0	3.692720	-0.817505	0.000072
7	7	0	-1.581259	0.864605	-0.000599
8	7	0	-0.783045	-1.469160	-0.000795
9	7	0	1.656959	-1.565213	-0.000716
10	7	0	2.130453	0.635818	0.000899
11	7	0	-3.085052	-0.904756	0.000880
12	1	0	-3.077299	-1.929002	0.001274
13	8	0	-0.160165	2.666695	-0.000524
14	1	0	1.796061	-2.565051	-0.000374
15	1	0	0.803952	2.799220	-0.000361

Guanine: 9H-trans-enol-guanine C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.968442336 A.U.
Zero-point correction= 0.102898
(Hartree/Particle)
Thermal correction to Energy= 0.110986
Thermal correction to Enthalpy= 0.111930
Thermal correction to Gibbs Free Energy= 0.070080
Sum of electronic and zero-point Energies= -541.865545
Sum of electronic and thermal Energies= -541.857458
Sum of electronic and thermal Enthalpies= -541.856513
Sum of electronic and thermal Free Energies= -541.898363

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.645	32.170	88.080

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.859572	0.382304	-0.009579
2	6	0	-0.472440	-0.968443	-0.007854
3	6	0	1.694607	-0.415601	-0.015469
4	6	0	0.184830	1.298448	-0.004708
5	6	0	-2.782028	-0.719699	0.011538
6	7	0	1.464123	0.913020	-0.008594
7	7	0	0.800188	-1.413495	-0.007496

8	7	0	-1.662568	-1.634206	0.007186
9	7	0	-2.239099	0.519923	0.001860
10	7	0	3.049105	-0.792559	-0.075387
11	1	0	3.661202	-0.087592	0.319230
12	1	0	3.207006	-1.715835	0.312254
13	8	0	-0.066756	2.639599	0.009930
14	1	0	-1.767775	-2.638185	0.008381
15	1	0	-1.041011	2.713983	0.014140

Guanine: 9H-trans-enol-guanine N9 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.030119958     A.U.
 Zero-point correction=                           0.103851
(Hartree/Particle)
 Thermal correction to Energy=                    0.111668
 Thermal correction to Enthalpy=                  0.112612
 Thermal correction to Gibbs Free Energy=         0.071190
 Sum of electronic and zero-point Energies=           -541.926269
 Sum of electronic and thermal Energies=              -541.918452
 Sum of electronic and thermal Enthalpies=            -541.917508
 Sum of electronic and thermal Free Energies=         -541.958931

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  70.073             30.932            87.182
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.839243	0.382371	-0.011819
2	6	0	-0.495886	-0.996995	-0.006418
3	6	0	1.686863	-0.444449	-0.015697
4	6	0	0.209358	1.295623	-0.005750
5	6	0	-2.600651	-0.759668	0.010379
6	1	0	-3.655316	-1.024779	0.019667
7	7	0	1.477068	0.898392	-0.009415
8	7	0	0.794561	-1.428425	-0.006010
9	7	0	-1.643258	-1.727696	0.007864
10	7	0	-2.210604	0.528275	0.000407
11	7	0	3.044715	-0.821655	-0.076728
12	1	0	3.653409	-0.128043	0.343075
13	1	0	3.191311	-1.752758	0.296903
14	8	0	-0.024328	2.645426	0.011085
15	1	0	-0.994805	2.738643	0.014670

Guanine: 9H-trans-enol-guanine OH deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.028432627     A.U.
```

```
 Zero-point correction=                           0.103100
(Hartree/Particle)
 Thermal correction to Energy=                    0.111150
 Thermal correction to Enthalpy=                  0.112094
 Thermal correction to Gibbs Free Energy=         0.070169
 Sum of electronic and zero-point Energies=           -541.925333
 Sum of electronic and thermal Energies=              -541.917283
 Sum of electronic and thermal Enthalpies=            -541.916339
 Sum of electronic and thermal Free Energies=         -541.958263

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.748             31.630             88.238

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.807624    0.503312   -0.005452
    2          6             0       -0.496820   -0.857913   -0.004560
    3          6             0        1.676447   -0.477689   -0.017665
    4          6             0        0.299791    1.454404   -0.002799
    5          6             0       -2.693153   -0.523170    0.007964
    6          1             0       -3.748479   -0.768994    0.013435
    7          7             0        1.557556    0.846446   -0.008027
    8          7             0        0.719972   -1.433644   -0.009185
    9          7             0       -1.716205   -1.509243    0.004557
   10          7             0       -2.187933    0.685702    0.003332
   11          7             0        2.996569   -0.970446   -0.075219
   12          1             0        3.660387   -0.294176    0.284666
   13          1             0        3.087003   -1.886588    0.349772
   14          8             0        0.173035    2.691886    0.010107
   15          1             0       -1.844762   -2.510701   -0.001848
 -------------------------------------------------------------------
```

Guanine: 9H-trans-enol-guanine OHa protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.864897076     A.U.
 Zero-point correction=                           0.127323
(Hartree/Particle)
 Thermal correction to Energy=                    0.136301
 Thermal correction to Enthalpy=                  0.137245
 Thermal correction to Gibbs Free Energy=         0.093702
 Sum of electronic and zero-point Energies=           -542.737574
 Sum of electronic and thermal Energies=              -542.728596
 Sum of electronic and thermal Enthalpies=            -542.727652
 Sum of electronic and thermal Free Energies=         -542.771196

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  85.530             35.400             91.645

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	0.831060	0.422860	-0.014388
2	6	0	0.500206	-0.963658	-0.003517
3	6	0	-1.712439	-0.579612	0.001195
4	6	0	-0.304683	1.185813	-0.016919
5	6	0	2.688922	-0.580652	0.007479
6	1	0	3.744980	-0.817210	0.018141
7	7	0	-1.528860	0.784288	-0.003010
8	7	0	-0.713960	-1.486139	-0.000086
9	7	0	1.725310	-1.577917	0.005997
10	7	0	2.193273	0.632979	-0.003574
11	7	0	-2.981490	-1.020424	0.013467
12	1	0	-3.755472	-0.372415	-0.018049
13	1	0	-3.164519	-2.014515	-0.000875
14	8	0	-0.164529	2.676392	-0.070864
15	1	0	1.889557	-2.578430	0.011100
16	1	0	0.680672	3.007054	0.316483
17	1	0	-0.957291	3.126366	0.307450

Guanine: 9H-trans-enol-guanine N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.938237449 A.U.
Zero-point correction= 0.129249
(Hartree/Particle)
Thermal correction to Energy= 0.137883
Thermal correction to Enthalpy= 0.138827
Thermal correction to Gibbs Free Energy= 0.095938
Sum of electronic and zero-point Energies= -542.808988
Sum of electronic and thermal Energies= -542.800355
Sum of electronic and thermal Enthalpies= -542.799410
Sum of electronic and thermal Free Energies= -542.842300

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.523	34.326	90.268

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.845738	0.442243	0.000064
2	6	0	-0.503699	-0.932271	0.000082
3	6	0	1.702795	-0.569181	0.000027
4	6	0	0.203857	1.336486	0.000106
5	6	0	-2.693513	-0.586662	-0.000118
6	1	0	-3.744617	-0.844671	-0.000155
7	7	0	1.463810	0.801035	0.000407
8	7	0	0.721758	-1.459221	-0.000017
9	7	0	-1.705954	-1.570004	0.000157
10	7	0	-2.214490	0.627940	-0.000266
11	7	0	2.981473	-0.979549	-0.000439
12	1	0	3.776314	-0.355703	-0.000097

13	1	0	3.158756	-1.976478	0.000297
14	8	0	0.159567	2.654059	-0.000084
15	1	0	-1.848866	-2.574329	0.000526
16	1	0	-0.765004	2.972955	-0.000159
17	1	0	2.238498	1.460660	0.000399

Guanine: 9H-trans-enol-guanine N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.929918065     A.U.
 Zero-point correction=                           0.129186
(Hartree/Particle)
 Thermal correction to Energy=                    0.137809
 Thermal correction to Enthalpy=                  0.138753
 Thermal correction to Gibbs Free Energy=         0.095899
 Sum of electronic and zero-point Energies=           -542.800732
 Sum of electronic and thermal Energies=              -542.792109
 Sum of electronic and thermal Enthalpies=            -542.791165
 Sum of electronic and thermal Free Energies=         -542.834019

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.476             34.438            90.193
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.824914	0.437855	0.000277
2	6	0	0.532863	-0.918164	0.000020
3	6	0	-1.760366	-0.420722	-0.000184
4	6	0	-0.266175	1.340410	-0.000015
5	6	0	2.703244	-0.556150	0.000198
6	1	0	3.757169	-0.800056	0.000424
7	7	0	-1.516290	0.884582	-0.000190
8	7	0	-0.757108	-1.374767	-0.000816
9	7	0	1.729059	-1.560366	-0.000128
10	7	0	2.188207	0.642239	0.000345
11	7	0	-3.034357	-0.836381	0.000792
12	1	0	-3.759002	-0.128099	0.000549
13	1	0	-3.315739	-1.807210	-0.000646
14	8	0	-0.114864	2.647796	-0.000282
15	1	0	1.907434	-2.558357	-0.000600
16	1	0	0.832397	2.890681	0.000019
17	1	0	-0.976801	-2.365843	0.000697

Guanine: 9H-trans-enol-guanine N7 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.925611489     A.U.
```

```
 Zero-point correction=                           0.129202
(Hartree/Particle)
 Thermal correction to Energy=                    0.137805
 Thermal correction to Enthalpy=                  0.138749
 Thermal correction to Gibbs Free Energy=         0.095911
 Sum of electronic and zero-point Energies=           -542.796410
 Sum of electronic and thermal Energies=              -542.787807
 Sum of electronic and thermal Enthalpies=            -542.786862
 Sum of electronic and thermal Free Energies=         -542.829701

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.474             34.423            90.161
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.753354	0.472245	-0.001560
2	6	0	-0.460700	-0.899784	-0.000409
3	6	0	1.725456	-0.546777	0.000104
4	6	0	0.373217	1.338263	-0.000358
5	6	0	-2.682174	-0.644088	0.000599
6	1	0	-3.740186	-0.863998	0.000944
7	7	0	1.570267	0.805689	0.000183
8	7	0	0.725362	-1.464340	0.000155
9	7	0	-1.695212	-1.552335	0.000390
10	7	0	-2.148067	0.578348	-0.000217
11	7	0	2.986123	-1.000091	0.000099
12	1	0	3.756654	-0.345611	-0.000415
13	1	0	3.170748	-1.993824	-0.000694
14	8	0	0.328380	2.676371	0.000587
15	1	0	-1.819036	-2.560589	0.001076
16	1	0	-0.572128	3.038577	0.002339
17	1	0	-2.707082	1.424435	-0.002478

Guanine: 9H-trans-enol-guanine N9H protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.870212597     A.U.
 Zero-point correction=                           0.128605
(Hartree/Particle)
 Thermal correction to Energy=                    0.137067
 Thermal correction to Enthalpy=                  0.138011
 Thermal correction to Gibbs Free Energy=         0.095435
 Sum of electronic and zero-point Energies=           -542.741608
 Sum of electronic and thermal Energies=              -542.733145
 Sum of electronic and thermal Enthalpies=            -542.732201
 Sum of electronic and thermal Free Energies=         -542.774778

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.011             34.066            89.610
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.748756	0.492463	0.000337
2	6	0	0.445476	-0.859017	0.000213
3	6	0	-1.733307	-0.532286	0.000044
4	6	0	-0.384068	1.345904	0.000517
5	6	0	2.741034	-0.372337	-0.000264
6	1	0	3.803624	-0.577488	-0.000437
7	7	0	-1.592374	0.808776	0.000217
8	7	0	-0.704732	-1.455094	0.000094
9	7	0	1.766999	-1.560438	0.000115
10	7	0	2.124057	0.736905	-0.000411
11	7	0	-2.975510	-1.026048	-0.000377
12	1	0	-3.765348	-0.393387	-0.000629
13	1	0	-3.133254	-2.024692	-0.000437
14	8	0	-0.314489	2.670069	-0.000145
15	1	0	1.883011	-2.162380	0.828896
16	1	0	0.608807	2.983317	-0.000523
17	1	0	1.882639	-2.162991	-0.828266

Guanine: 9H-trans-enol-guanine N2 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.914805985 A.U.
Zero-point correction= 0.131098
(Hartree/Particle)
Thermal correction to Energy= 0.139534
Thermal correction to Enthalpy= 0.140478
Thermal correction to Gibbs Free Energy= 0.097448
Sum of electronic and zero-point Energies= -542.783708
Sum of electronic and thermal Energies= -542.775272
Sum of electronic and thermal Enthalpies= -542.774328
Sum of electronic and thermal Free Energies= -542.817358

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.559	32.585	90.566

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856578	0.421496	0.000039
2	6	0	-0.501310	-0.939956	0.000009
3	6	0	1.609129	-0.407631	-0.000033
4	6	0	0.194921	1.356025	-0.000037
5	6	0	-2.686964	-0.648666	-0.000005
6	1	0	-3.734681	-0.919982	-0.000049
7	7	0	1.459947	0.902487	-0.000037
8	7	0	0.760979	-1.411763	-0.000043
9	7	0	-1.691421	-1.610814	-0.000080
10	7	0	-2.222513	0.578409	0.000069

11	7	0	3.047629	-0.831125	0.000040
12	1	0	3.536321	-0.464044	0.827777
13	1	0	3.104078	-1.858012	-0.000635
14	8	0	0.032319	2.668395	-0.000004
15	1	0	-1.820671	-2.616254	0.000312
16	1	0	-0.917879	2.895983	0.000037
17	1	0	3.536735	-0.462819	-0.826898

Guanine: NEUTRAL 9H-cis-enol-guanine
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.573126021     A.U.
 Zero-point correction=                           0.116678
(Hartree/Particle)
 Thermal correction to Energy=                    0.124824
 Thermal correction to Enthalpy=                  0.125768
 Thermal correction to Gibbs Free Energy=         0.083861
 Sum of electronic and zero-point Energies=           -542.456448
 Sum of electronic and thermal Energies=              -542.448302
 Sum of electronic and thermal Enthalpies=            -542.447358
 Sum of electronic and thermal Free Energies=         -542.489265

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  78.328             32.792             88.201
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.815137	0.486471	-0.003608
2	6	0	-0.529720	-0.891499	0.000385
3	6	0	1.666947	-0.569136	-0.005025
4	6	0	0.321371	1.309910	-0.000371
5	6	0	-2.707964	-0.483463	0.001586
6	1	0	-3.768103	-0.701271	0.002437
7	7	0	1.541169	0.781745	-0.001057
8	7	0	0.673499	-1.470331	0.003066
9	7	0	-1.761878	-1.499040	0.003918
10	7	0	-2.184189	0.713922	-0.002129
11	7	0	2.950729	-1.050467	-0.059667
12	1	0	3.688672	-0.410702	0.198417
13	1	0	3.079866	-2.021990	0.186770
14	8	0	0.208290	2.647260	0.005401
15	1	0	-1.929808	-2.495931	0.001376
16	1	0	1.114758	3.007314	0.001065

Guanine: 9H-cis-enol-guanine N2Ha deprotonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.993257812     A.U.
```

```
 Zero-point correction=                           0.102264
(Hartree/Particle)
 Thermal correction to Energy=                    0.110313
 Thermal correction to Enthalpy=                  0.111257
 Thermal correction to Gibbs Free Energy=         0.069205
 Sum of electronic and zero-point Energies=           -541.890994
 Sum of electronic and thermal Energies=              -541.882945
 Sum of electronic and thermal Enthalpies=            -541.882001
 Sum of electronic and thermal Free Energies=         -541.924053

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.223             31.622             88.507

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0        0.757361    0.514449    0.000379
    2          6             0        0.529048   -0.883418   -0.000283
    3          6             0       -1.739362   -0.732546   -0.000030
    4          6             0       -0.437378    1.258373   -0.000055
    5          6             0        2.708550   -0.354798    0.000262
    6          1             0        3.780032   -0.514281    0.000172
    7          7             0       -1.614065    0.684167   -0.000396
    8          7             0       -0.606723   -1.545729   -0.000626
    9          7             0        1.812456   -1.419667   -0.000685
   10          7             0        2.117075    0.813299    0.000696
   11          7             0       -2.926130   -1.285282    0.000749
   12          1             0       -3.607836   -0.522478    0.001110
   13          8             0       -0.404486    2.628014   -0.000240
   14          1             0        2.023426   -2.406733    0.001411
   15          1             0       -1.347341    2.879511   -0.000568
 -----------------------------------------------------------------------
```

Guanine: 9H-cis-enol-guanine N2Hb deprotonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.993900351     A.U.
 Zero-point correction=                           0.102301
(Hartree/Particle)
 Thermal correction to Energy=                    0.110344
 Thermal correction to Enthalpy=                  0.111288
 Thermal correction to Gibbs Free Energy=         0.069234
 Sum of electronic and zero-point Energies=           -541.891600
 Sum of electronic and thermal Energies=              -541.883557
 Sum of electronic and thermal Enthalpies=            -541.882613
 Sum of electronic and thermal Free Energies=         -541.924667

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.242             31.572             88.511

-----------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.767637	0.502216	0.000151
2	6	0	0.499977	-0.886044	-0.000263
3	6	0	-1.773147	-0.647575	0.000045
4	6	0	-0.407878	1.282529	-0.000010
5	6	0	2.693667	-0.423454	0.000353
6	1	0	3.759812	-0.614847	0.000342
7	7	0	-1.601004	0.751931	-0.000201
8	7	0	-0.662692	-1.507234	-0.000378
9	7	0	1.765069	-1.461636	-0.000716
10	7	0	2.134970	0.760748	0.000483
11	7	0	-3.001186	-1.100934	0.000486
12	1	0	-2.931811	-2.122655	0.000707
13	8	0	-0.329774	2.649674	-0.000187
14	1	0	1.948142	-2.454172	0.001343
15	1	0	-1.265588	2.928128	-0.000277

Guanine: 9H-cis-enol-guanine C8 deprotonation
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.962595852 A.U.
Zero-point correction= 0.102472
(Hartree/Particle)
Thermal correction to Energy= 0.110625
Thermal correction to Enthalpy= 0.111569
Thermal correction to Gibbs Free Energy= 0.069615
Sum of electronic and zero-point Energies= -541.860124
Sum of electronic and thermal Energies= -541.851971
Sum of electronic and thermal Enthalpies= -541.851027
Sum of electronic and thermal Free Energies= -541.892981

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.418	32.469	88.300

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.884065	0.461704	-0.005373
2	6	0	-0.559589	-0.920151	-0.005959
3	6	0	1.640704	-0.530927	-0.015608
4	6	0	0.231725	1.292362	-0.003498
5	6	0	-2.850593	-0.570032	0.010799
6	7	0	1.486683	0.805081	-0.008550
7	7	0	0.677360	-1.455565	-0.008221
8	7	0	-1.770579	-1.533501	0.004459
9	7	0	-2.261363	0.643127	0.005415
10	7	0	2.968107	-0.997954	-0.076530
11	1	0	3.624789	-0.347784	0.340268
12	1	0	3.054925	-1.935074	0.300949
13	8	0	0.126814	2.652251	0.007775
14	1	0	-1.911431	-2.533240	0.001798

15	1	0	1.046661	2.972042	-0.003400

Guanine: 9H-cis-enol-guanine N9 deprotonation
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.027306809 A.U.
Zero-point correction= 0.103639
(Hartree/Particle)
Thermal correction to Energy= 0.111471
Thermal correction to Enthalpy= 0.112415
Thermal correction to Gibbs Free Energy= 0.070977
Sum of electronic and zero-point Energies= -541.923668
Sum of electronic and thermal Energies= -541.915836
Sum of electronic and thermal Enthalpies= -541.914892
Sum of electronic and thermal Free Energies= -541.956330

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.949	31.028	87.214

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.860671	0.452016	-0.006613
2	6	0	-0.578405	-0.955165	-0.005757
3	6	0	1.635550	-0.548531	-0.015937
4	6	0	0.249498	1.288136	-0.003792
5	6	0	-2.665590	-0.624753	0.009721
6	1	0	-3.730539	-0.847069	0.017238
7	7	0	1.495877	0.800190	-0.009649
8	7	0	0.682376	-1.467486	-0.007063
9	7	0	-1.749946	-1.635704	0.005098
10	7	0	-2.227669	0.641784	0.003777
11	7	0	2.969639	-1.007368	-0.077845
12	1	0	3.616563	-0.367160	0.369364
13	1	0	3.048949	-1.952384	0.281915
14	8	0	0.141065	2.651018	0.008541
15	1	0	1.062271	2.968341	-0.002793

Guanine: 9H-cis-enol-guanine OH deprotonation
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.028432143 A.U.
Zero-point correction= 0.103099
(Hartree/Particle)
Thermal correction to Energy= 0.111148
Thermal correction to Enthalpy= 0.112092
Thermal correction to Gibbs Free Energy= 0.070170
Sum of electronic and zero-point Energies= -541.925333

```
 Sum of electronic and thermal Energies=             -541.917284
 Sum of electronic and thermal Enthalpies=           -541.916340
 Sum of electronic and thermal Free Energies=        -541.958262

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.747             31.629             88.233

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.807779    0.503269   -0.005347
    2          6             0       -0.496440   -0.857902   -0.004321
    3          6             0        1.676604   -0.477224   -0.016845
    4          6             0        0.299185    1.454284   -0.002262
    5          6             0       -2.692951   -0.523765    0.007757
    6          1             0       -3.748213   -0.769870    0.013026
    7          7             0        1.557347    0.846909   -0.007735
    8          7             0        0.720318   -1.433454   -0.008589
    9          7             0       -1.715725   -1.509516    0.004530
   10          7             0       -2.188164    0.685257    0.002763
   11          7             0        2.996790   -0.969925   -0.076011
   12          1             0        3.661535   -0.294054    0.283069
   13          1             0        3.088006   -1.886556    0.347920
   14          8             0        0.172113    2.691828    0.009897
   15          1             0       -1.843915   -2.511013   -0.001791
 -------------------------------------------------------------------
```

Guanine: 9H-cis-enol-guanine OHb protonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.864897280     A.U.
 Zero-point correction=                           0.127324
(Hartree/Particle)
 Thermal correction to Energy=                    0.136302
 Thermal correction to Enthalpy=                  0.137247
 Thermal correction to Gibbs Free Energy=         0.093702
 Sum of electronic and zero-point Energies=           -542.737573
 Sum of electronic and thermal Energies=              -542.728595
 Sum of electronic and thermal Enthalpies=            -542.727651
 Sum of electronic and thermal Free Energies=         -542.771195

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  85.531             35.399             91.647

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.831094    0.422975   -0.014393
    2          6             0        0.500434   -0.963567   -0.003495
    3          6             0       -1.712235   -0.580073    0.001183
```

4	6	0	-0.304917	1.185640	-0.016889
5	6	0	2.689090	-0.580326	0.007507
6	1	0	3.745195	-0.816658	0.018141
7	7	0	-1.528897	0.783860	-0.002966
8	7	0	-0.713704	-1.486305	0.000022
9	7	0	1.725591	-1.577657	0.006072
10	7	0	2.193236	0.633252	-0.003831
11	7	0	-2.981177	-1.020923	0.012770
12	1	0	-3.755077	-0.372794	-0.015775
13	1	0	-3.164212	-2.014973	0.000668
14	8	0	-0.165206	2.676925	-0.070910
15	1	0	1.889858	-2.578166	0.011217
16	1	0	-0.959030	3.125955	0.306234
17	1	0	0.678771	3.007753	0.318854

Guanine: 9H-cis-enol-guanine N1 protonation
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.923799582 A.U.
Zero-point correction= 0.128066
(Hartree/Particle)
Thermal correction to Energy= 0.137231
Thermal correction to Enthalpy= 0.138175
Thermal correction to Gibbs Free Energy= 0.093798
Sum of electronic and zero-point Energies= -542.795734
Sum of electronic and thermal Energies= -542.786569
Sum of electronic and thermal Enthalpies= -542.785625
Sum of electronic and thermal Free Energies= -542.830001

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.113	35.247	93.398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.849844	0.463798	0.000005
2	6	0	0.525092	-0.919122	0.000047
3	6	0	-1.686109	-0.604016	0.000020
4	6	0	-0.215632	1.342988	0.000008
5	6	0	2.706758	-0.551932	-0.000030
6	1	0	3.760264	-0.800352	-0.000054
7	7	0	-1.471543	0.775061	0.000121
8	7	0	-0.691461	-1.470488	0.000089
9	7	0	1.728441	-1.546975	0.000024
10	7	0	2.218110	0.656325	-0.000074
11	7	0	-2.959789	-1.035765	-0.000432
12	1	0	-3.768003	-0.429850	0.001224
13	1	0	-3.117610	-2.036045	0.000384
14	8	0	-0.055160	2.651799	0.000049
15	1	0	1.877082	-2.550348	0.000070
16	1	0	-0.874832	3.176973	-0.000644

17	1	0	-2.281650	1.387815	0.000242

Guanine: 9H-cis-enol-guanine N3 protonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.930644653     A.U.
 Zero-point correction=                           0.129081
(Hartree/Particle)
 Thermal correction to Energy=                    0.137722
 Thermal correction to Enthalpy=                  0.138666
 Thermal correction to Gibbs Free Energy=         0.095784
 Sum of electronic and zero-point Energies=           -542.801563
 Sum of electronic and thermal Energies=              -542.792923
 Sum of electronic and thermal Enthalpies=            -542.791979
 Sum of electronic and thermal Free Energies=         -542.834860

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.422             34.509             90.251
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.837351	0.479447	-0.000176
2	6	0	-0.578136	-0.888322	0.000021
3	6	0	1.733592	-0.484717	-0.000042
4	6	0	0.291474	1.332597	-0.000036
5	6	0	-2.735737	-0.476608	-0.000069
6	1	0	-3.794759	-0.697918	-0.000142
7	7	0	1.529927	0.828971	0.000023
8	7	0	0.695519	-1.392318	0.000289
9	7	0	-1.784399	-1.505729	0.000105
10	7	0	-2.197605	0.708736	-0.000232
11	7	0	2.992183	-0.947218	-0.000267
12	1	0	3.746391	-0.271416	-0.000245
13	1	0	3.233777	-1.928711	0.000073
14	8	0	0.128796	2.635660	0.000213
15	1	0	-1.982603	-2.499823	0.000267
16	1	0	0.998727	3.082472	0.000301
17	1	0	0.875683	-2.391363	0.000425

Guanine: 9H-cis-enol-guanine N7 protonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.943236419     A.U.
 Zero-point correction=                           0.130075
(Hartree/Particle)
 Thermal correction to Energy=                    0.138370
 Thermal correction to Enthalpy=                  0.139314
 Thermal correction to Gibbs Free Energy=         0.097105
 Sum of electronic and zero-point Energies=           -542.813162
```

```
 Sum of electronic and thermal Energies=             -542.804867
 Sum of electronic and thermal Enthalpies=           -542.803922
 Sum of electronic and thermal Free Energies=        -542.846131

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.828             33.654             88.836

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.752506    0.467555   -0.000892
    2          6             0       -0.475286   -0.901582   -0.000326
    3          6             0        1.718663   -0.560356   -0.000028
    4          6             0        0.369397    1.323086   -0.000391
    5          6             0       -2.692375   -0.603061    0.000557
    6          1             0       -3.753722   -0.805716    0.000891
    7          7             0        1.573982    0.800497    0.000037
    8          7             0        0.713943   -1.468989   -0.000068
    9          7             0       -1.720076   -1.533085    0.000041
   10          7             0       -2.135703    0.607490    0.000026
   11          7             0        2.976860   -1.022938    0.000346
   12          1             0        3.755465   -0.378853    0.000041
   13          1             0        3.150855   -2.018641   -0.000149
   14          8             0        0.180593    2.641417    0.000298
   15          1             0       -1.865902   -2.538147    0.000168
   16          1             0        1.048077    3.092290    0.000962
   17          1             0       -2.649917    1.483054   -0.000507
 -------------------------------------------------------------------
```

Guanine: 9H-cis-enol-guanine N9H protonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.876120970     A.U.
 Zero-point correction=                           0.128741
(Hartree/Particle)
 Thermal correction to Energy=                    0.137165
 Thermal correction to Enthalpy=                  0.138109
 Thermal correction to Gibbs Free Energy=         0.095604
 Sum of electronic and zero-point Energies=           -542.747380
 Sum of electronic and thermal Energies=              -542.738956
 Sum of electronic and thermal Enthalpies=            -542.738012
 Sum of electronic and thermal Free Energies=         -542.780517

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.072             33.948             89.460

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
```

1	6	0	0.755026	0.521484	0.000209
2	6	0	0.483801	-0.836668	0.000114
3	6	0	-1.707494	-0.584462	0.000069
4	6	0	-0.404856	1.333598	0.000574
5	6	0	2.764374	-0.297793	-0.000159
6	1	0	3.830681	-0.483529	-0.000243
7	7	0	-1.602499	0.763234	0.000251
8	7	0	-0.652370	-1.466632	0.000101
9	7	0	1.814949	-1.511399	0.000102
10	7	0	2.127130	0.796552	-0.000431
11	7	0	-2.935475	-1.115085	-0.000334
12	1	0	-3.747064	-0.511525	-0.000653
13	1	0	-3.059850	-2.118450	-0.000471
14	8	0	-0.291753	2.649899	-0.000163
15	1	0	1.943112	-2.110403	0.828932
16	1	0	-1.183016	3.051891	-0.000484
17	1	0	1.942907	-2.110819	-0.828455

Guanine: 9H-cis-enol-guanine N2 protonation
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.912903070     A.U.
 Zero-point correction=                           0.130945
(Hartree/Particle)
 Thermal correction to Energy=                    0.139383
 Thermal correction to Enthalpy=                  0.140327
 Thermal correction to Gibbs Free Energy=         0.097357
 Sum of electronic and zero-point Energies=           -542.781958
 Sum of electronic and thermal Energies=              -542.773520
 Sum of electronic and thermal Enthalpies=            -542.772576
 Sum of electronic and thermal Free Energies=         -542.815546
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.464	32.689	90.438

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.869566	0.458612	0.000024
2	6	0	0.543720	-0.915245	0.000002
3	6	0	-1.586625	-0.458079	-0.000083
4	6	0	-0.218272	1.352805	0.000080
5	6	0	2.718672	-0.579611	-0.000019
6	1	0	3.771666	-0.830090	0.000019
7	7	0	-1.472712	0.858895	-0.000057
8	7	0	-0.704155	-1.426892	-0.000017
9	7	0	1.743005	-1.563697	0.000067
10	7	0	2.232437	0.637034	0.000061
11	7	0	-3.007507	-0.934802	0.000051
12	1	0	-3.513379	-0.592293	-0.827787
13	1	0	-3.016736	-1.963539	-0.000547
14	8	0	-0.028896	2.659467	-0.000041
15	1	0	1.889195	-2.566635	-0.000614

16	1	0	-0.886537	3.125515	-0.000132
17	1	0	-3.512883	-0.593347	0.828631

Guanine: NEUTRAL 7H-trans-enol-guanine
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.555031504 A.U.
Zero-point correction= 0.115353
(Hartree/Particle)
Thermal correction to Energy= 0.124075
Thermal correction to Enthalpy= 0.125019
Thermal correction to Gibbs Free Energy= 0.081856
Sum of electronic and zero-point Energies= -542.439679
Sum of electronic and thermal Energies= -542.430957
Sum of electronic and thermal Enthalpies= -542.430013
Sum of electronic and thermal Free Energies= -542.473175

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.858	33.930	90.843

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787552	0.418503	-0.014815
2	6	0	-0.486277	-0.962025	0.001660
3	6	0	1.706140	-0.500039	-0.005423
4	6	0	0.290988	1.311171	-0.001150
5	6	0	-2.617738	-0.814078	0.002806
6	1	0	-3.675372	-1.046896	0.002733
7	7	0	1.523354	0.846677	-0.001042
8	7	0	0.760840	-1.445998	0.008359
9	7	0	-1.654127	-1.703850	0.013154
10	7	0	-2.179047	0.486826	-0.006648
11	7	0	3.012737	-0.916353	-0.064121
12	1	0	3.718595	-0.240334	0.191531
13	1	0	3.187927	-1.881516	0.178812
14	8	0	0.177056	2.667419	0.011782
15	1	0	-0.754477	2.934778	0.039250
16	1	0	-2.772788	1.302316	-0.052974

Guanine: 7H-trans-enol-guanine N2Ha deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.966547586 A.U.
Zero-point correction= 0.101562
(Hartree/Particle)
Thermal correction to Energy= 0.109785
Thermal correction to Enthalpy= 0.110729
Thermal correction to Gibbs Free Energy= 0.068231

```
 Sum of electronic and zero-point Energies=          -541.864986
 Sum of electronic and thermal Energies=             -541.856763
 Sum of electronic and thermal Enthalpies=           -541.855819
 Sum of electronic and thermal Free Energies=        -541.898317

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  68.891             31.937             89.446

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.715797    0.409079    0.187682
    2          6             0        0.447208   -0.969074   -0.009194
    3          6             0       -1.811634   -0.609868   -0.002852
    4          6             0       -0.385561    1.260666   -0.000377
    5          6             0        2.597085   -0.735505   -0.014076
    6          1             0        3.665667   -0.927999   -0.006078
    7          7             0       -1.595521    0.797858   -0.077640
    8          7             0       -0.746862   -1.504230   -0.128428
    9          7             0        1.682222   -1.656944   -0.120929
   10          7             0        2.122615    0.564621    0.087139
   11          7             0       -3.025721   -1.072536    0.141159
   12          1             0       -3.646429   -0.260064    0.184969
   13          8             0       -0.226255    2.638273   -0.102544
   14          1             0        0.712924    2.812424   -0.275675
   15          1             0        2.643385    1.236284    0.640934
 ---------------------------------------------------------------------
```

Guanine: 7H-trans-enol-guanine N2Hb deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.967478288     A.U.
 Zero-point correction=                           0.101582
(Hartree/Particle)
 Thermal correction to Energy=                    0.109827
 Thermal correction to Enthalpy=                  0.110771
 Thermal correction to Gibbs Free Energy=         0.068211
 Sum of electronic and zero-point Energies=          -541.865896
 Sum of electronic and thermal Energies=             -541.857652
 Sum of electronic and thermal Enthalpies=           -541.856707
 Sum of electronic and thermal Free Energies=        -541.899267

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  68.917             31.959             89.575

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.726569    0.397129    0.171198
    2          6             0        0.413387   -0.969441   -0.015484
```

3	6	0	-1.841185	-0.515365	-0.001411
4	6	0	-0.350889	1.287721	0.001260
5	6	0	2.568958	-0.812413	-0.009829
6	1	0	3.629829	-1.042164	0.003348
7	7	0	-1.574963	0.872886	-0.065434
8	7	0	-0.805746	-1.456333	-0.129233
9	7	0	1.620069	-1.702220	-0.116495
10	7	0	2.136812	0.500236	0.082929
11	7	0	-3.089850	-0.876669	0.138676
12	1	0	-3.090936	-1.900754	0.150390
13	8	0	-0.140724	2.659787	-0.090968
14	1	0	0.799835	2.800889	-0.284350
15	1	0	2.681776	1.172646	0.610849

Guanine: 7H-trans-enol-guanine N7 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.030119985 A.U.
Zero-point correction= 0.103850
(Hartree/Particle)
Thermal correction to Energy= 0.111669
Thermal correction to Enthalpy= 0.112613
Thermal correction to Gibbs Free Energy= 0.071188
Sum of electronic and zero-point Energies= -541.926270
Sum of electronic and thermal Energies= -541.918451
Sum of electronic and thermal Enthalpies= -541.917507
Sum of electronic and thermal Free Energies= -541.958932

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.073	30.935	87.187

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.839359	0.382426	-0.011856
2	6	0	-0.495828	-0.996946	-0.006449
3	6	0	1.686896	-0.444431	-0.016008
4	6	0	0.209214	1.295634	-0.005808
5	6	0	-2.600598	-0.759877	0.010517
6	1	0	-3.655296	-1.024859	0.019768
7	7	0	1.476962	0.898380	-0.009562
8	7	0	0.794654	-1.428405	-0.006137
9	7	0	-1.643058	-1.727660	0.007873
10	7	0	-2.210877	0.528182	0.000441
11	7	0	3.044808	-0.821564	-0.076452
12	1	0	3.653345	-0.128075	0.343790
13	1	0	3.191284	-1.752789	0.296940
14	8	0	-0.024257	2.645417	0.011135
15	1	0	-0.994656	2.739023	0.014909

Guanine: 7H-trans-enol-guanine C8 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.955711841     A.U.
 Zero-point correction=                           0.101476
(Hartree/Particle)
 Thermal correction to Energy=                    0.110095
 Thermal correction to Enthalpy=                  0.111040
 Thermal correction to Gibbs Free Energy=         0.068049
 Sum of electronic and zero-point Energies=           -541.854236
 Sum of electronic and thermal Energies=              -541.845616
 Sum of electronic and thermal Enthalpies=            -541.844672
 Sum of electronic and thermal Free Energies=         -541.887663

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.086             33.321             90.481

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0       -0.841169    0.386182   -0.023178
    2          6             0       -0.509395   -0.999176   -0.004774
    3          6             0        1.681570   -0.443462   -0.016338
    4          6             0        0.202487    1.292612   -0.005972
    5          6             0       -2.729993   -0.940664    0.011402
    6          7             0        1.473569    0.891060   -0.010139
    7          7             0        0.778321   -1.420999   -0.001928
    8          7             0       -1.639272   -1.760468    0.016897
    9          7             0       -2.231763    0.384371    0.000878
   10          7             0        3.031902   -0.835162   -0.079340
   11          1             0        3.655064   -0.149890    0.332159
   12          1             0        3.170266   -1.770375    0.286540
   13          8             0        0.029168    2.663800    0.016665
   14          1             0       -0.923547    2.842392    0.050843
   15          1             0       -2.845431    1.182914   -0.054277
 -----------------------------------------------------------------------
```

Guanine: 7H-trans-enol-guanine OH deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.033153946     A.U.
 Zero-point correction=                           0.103458
(Hartree/Particle)
 Thermal correction to Energy=                    0.111428
 Thermal correction to Enthalpy=                  0.112372
 Thermal correction to Gibbs Free Energy=         0.070617
 Sum of electronic and zero-point Energies=           -541.929697
 Sum of electronic and thermal Energies=              -541.921727
 Sum of electronic and thermal Enthalpies=            -541.920783
 Sum of electronic and thermal Free Energies=         -541.962537
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.922	31.355	87.880

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.767427	0.420652	-0.012101
2	6	0	-0.478974	-0.942013	-0.006423
3	6	0	1.695006	-0.436203	-0.016920
4	6	0	0.261288	1.429805	-0.003562
5	6	0	-2.618419	-0.774085	0.010516
6	1	0	-3.679257	-0.995566	0.018825
7	7	0	1.531867	0.899261	-0.007421
8	7	0	0.789456	-1.424872	-0.008242
9	7	0	-1.657033	-1.681931	0.007132
10	7	0	-2.148568	0.509594	0.001263
11	7	0	3.039837	-0.860003	-0.075668
12	1	0	3.668963	-0.166306	0.312229
13	1	0	3.165648	-1.783940	0.322574
14	8	0	0.010007	2.661247	0.012571
15	1	0	-2.673173	1.372552	-0.002702

Guanine: 7H-trans-enol-guanine OHa protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.843978760 A.U.
Zero-point correction= 0.126351
(Hartree/Particle)
Thermal correction to Energy= 0.135703
Thermal correction to Enthalpy= 0.136647
Thermal correction to Gibbs Free Energy= 0.092173
Sum of electronic and zero-point Energies= -542.717627
Sum of electronic and thermal Energies= -542.708276
Sum of electronic and thermal Enthalpies= -542.707331
Sum of electronic and thermal Free Energies= -542.751806

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.155	36.097	93.604

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.826272	0.438300	-0.007207
2	6	0	-0.550616	-0.983817	0.019215
3	6	0	1.689404	-0.631878	0.000761
4	6	0	0.321786	1.170549	-0.002691
5	6	0	-2.673102	-0.751256	-0.013355
6	1	0	-3.737219	-0.952953	-0.030099
7	7	0	1.537653	0.733959	-0.006162

8	7	0	0.666988	-1.501551	0.024996
9	7	0	-1.740177	-1.669580	0.018563
10	7	0	-2.201112	0.544712	-0.021716
11	7	0	2.945440	-1.111082	-0.012502
12	1	0	3.742497	-0.491810	-0.027691
13	1	0	3.090937	-2.111652	-0.007100
14	8	0	0.267159	2.706435	-0.037119
15	1	0	0.160820	3.092375	0.863306
16	1	0	-2.765164	1.379983	-0.112411
17	1	0	1.142108	3.005988	-0.391648

Guanine: 7H-trans-enol-guanine N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.919803845 A.U.
Zero-point correction= 0.127988
(Hartree/Particle)
Thermal correction to Energy= 0.137101
Thermal correction to Enthalpy= 0.138045
Thermal correction to Gibbs Free Energy= 0.094156
Sum of electronic and zero-point Energies= -542.791816
Sum of electronic and thermal Energies= -542.782703
Sum of electronic and thermal Enthalpies= -542.781759
Sum of electronic and thermal Free Energies= -542.825648

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.032	35.427	92.373

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.834777	0.436928	0.000428
2	6	0	-0.524463	-0.964758	0.000107
3	6	0	1.698279	-0.582903	0.000000
4	6	0	0.208042	1.330167	0.000073
5	6	0	-2.646398	-0.807043	-0.000134
6	1	0	-3.702093	-1.050204	-0.000265
7	7	0	1.464559	0.786094	0.000029
8	7	0	0.714704	-1.462838	-0.000090
9	7	0	-1.675352	-1.695366	-0.000220
10	7	0	-2.220897	0.494703	0.000014
11	7	0	2.975031	-1.001123	0.000122
12	1	0	3.776075	-0.385516	-0.000198
13	1	0	3.139275	-2.000663	0.000025
14	8	0	0.227608	2.661555	-0.000403
15	1	0	-0.656081	3.066308	0.000727
16	1	0	-2.826299	1.305890	0.001192
17	1	0	2.237853	1.447113	-0.000088

Guanine: 7H-trans-enol-guanine N2 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.903275526     A.U.
 Zero-point correction=                           0.130267
(Hartree/Particle)
 Thermal correction to Energy=                    0.138961
 Thermal correction to Enthalpy=                  0.139905
 Thermal correction to Gibbs Free Energy=         0.096444
 Sum of electronic and zero-point Energies=           -542.773009
 Sum of electronic and thermal Energies=              -542.764314
 Sum of electronic and thermal Enthalpies=            -542.763370
 Sum of electronic and thermal Free Energies=         -542.806832

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.845332	0.410894	0.000025
2	6	0	0.519344	-0.971916	0.000025
3	6	0	-1.605793	-0.416628	-0.000022
4	6	0	-0.197111	1.351354	0.000025
5	6	0	2.635351	-0.876790	-0.000007
6	1	0	3.686065	-1.138402	-0.000031
7	7	0	-1.455802	0.895846	-0.000003
8	7	0	-0.760498	-1.411087	-0.000004
9	7	0	1.644421	-1.741197	-0.000007
10	7	0	2.226251	0.434991	-0.000005
11	7	0	-3.043531	-0.846302	0.000000
12	1	0	-3.537280	-0.486462	-0.827563
13	1	0	-3.081995	-1.874699	-0.001019
14	8	0	-0.084104	2.682109	-0.000041
15	1	0	0.837599	2.988443	0.000216
16	1	0	2.846579	1.235204	-0.000031
17	1	0	-3.536771	-0.488200	0.828620

Guanine: 7H-trans-enol-guanine N3 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.931772210     A.U.
 Zero-point correction=                           0.129089
(Hartree/Particle)
 Thermal correction to Energy=                    0.137770
 Thermal correction to Enthalpy=                  0.138714
 Thermal correction to Gibbs Free Energy=         0.095724
 Sum of electronic and zero-point Energies=           -542.802684
 Sum of electronic and thermal Energies=              -542.794003
 Sum of electronic and thermal Enthalpies=            -542.793058
 Sum of electronic and thermal Free Energies=         -542.836048
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.452	34.601	90.480

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.821418	0.439869	-0.000569
2	6	0	0.550717	-0.929685	-0.000056
3	6	0	-1.751621	-0.444973	-0.000046
4	6	0	-0.269731	1.338940	-0.000096
5	6	0	2.650984	-0.794703	0.000128
6	1	0	3.704550	-1.042346	0.000236
7	7	0	-1.508536	0.866115	0.000020
8	7	0	-0.744137	-1.373772	-0.000218
9	7	0	1.666984	-1.685027	0.000321
10	7	0	2.211216	0.494618	-0.000203
11	7	0	-3.025760	-0.857511	0.000202
12	1	0	-3.752890	-0.152360	-0.000779
13	1	0	-3.300840	-1.830399	-0.001058
14	8	0	-0.184721	2.665446	0.000347
15	1	0	0.728454	2.997921	0.000815
16	1	0	2.810195	1.311295	-0.000915
17	1	0	-0.920669	-2.375323	0.001901

Guanine: 7H-trans-enol-guanine N7H protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.853602046     A.U.
 Zero-point correction=                           0.128055
(Hartree/Particle)
 Thermal correction to Energy=                    0.136774
 Thermal correction to Enthalpy=                  0.137718
 Thermal correction to Gibbs Free Energy=         0.094519
 Sum of electronic and zero-point Energies=           -542.725547
 Sum of electronic and thermal Energies=              -542.716829
 Sum of electronic and thermal Enthalpies=            -542.715885
 Sum of electronic and thermal Free Energies=         -542.759084
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.827	34.469	90.919

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.734610	0.434638	-0.003799
2	6	0	-0.442209	-0.936981	-0.001453
3	6	0	1.746728	-0.517747	0.000261
4	6	0	0.353945	1.325479	-0.000581
5	6	0	-2.623238	-0.926330	0.001727

6	1	0	-3.687752	-1.133095	0.003118
7	7	0	1.572634	0.822969	0.000634
8	7	0	0.750363	-1.459013	-0.000187
9	7	0	-1.645713	-1.711264	0.000627
10	7	0	-2.195411	0.571949	-0.000142
11	7	0	3.002101	-0.975754	0.000309
12	1	0	3.778893	-0.327946	0.000983
13	1	0	3.177389	-1.971884	0.000234
14	8	0	0.291173	2.664654	0.001285
15	1	0	-0.612657	3.018500	-0.001269
16	1	0	-2.590538	1.039671	-0.831044
17	1	0	-2.586232	1.040958	0.832079

Guanine: 7H-trans-enol-guanine N9 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.925611732 A.U.
Zero-point correction= 0.129202
(Hartree/Particle)
Thermal correction to Energy= 0.137805
Thermal correction to Enthalpy= 0.138749
Thermal correction to Gibbs Free Energy= 0.095911
Sum of electronic and zero-point Energies= -542.796410
Sum of electronic and thermal Energies= -542.787807
Sum of electronic and thermal Enthalpies= -542.786862
Sum of electronic and thermal Free Energies= -542.829701

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.474	34.423	90.161

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.753391	0.472274	0.000275
2	6	0	-0.460732	-0.899745	0.000182
3	6	0	1.725460	-0.546998	-0.000074
4	6	0	0.373291	1.338290	-0.000025
5	6	0	-2.682125	-0.644122	-0.000180
6	1	0	-3.740153	-0.863918	-0.000251
7	7	0	1.570265	0.805707	-0.000153
8	7	0	0.725322	-1.464334	0.000032
9	7	0	-1.695134	-1.552334	-0.000110
10	7	0	-2.148103	0.578376	0.000123
11	7	0	2.986085	-1.000003	0.000028
12	1	0	3.756367	-0.345257	0.000021
13	1	0	3.170984	-1.993669	0.000241
14	8	0	0.328369	2.676312	-0.000241
15	1	0	-0.572153	3.038471	0.001754
16	1	0	-2.707213	1.424403	-0.000406
17	1	0	-1.818837	-2.560604	0.000061

Guanine: NEUTRAL 7H-cis-enol-guanine
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.568468621     A.U.
 Zero-point correction=                           0.116399
(Hartree/Particle)
 Thermal correction to Energy=                    0.124646
 Thermal correction to Enthalpy=                  0.125590
 Thermal correction to Gibbs Free Energy=         0.083495
 Sum of electronic and zero-point Energies=           -542.452070
 Sum of electronic and thermal Energies=              -542.443823
 Sum of electronic and thermal Enthalpies=            -542.442879
 Sum of electronic and thermal Free Energies=         -542.484974

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  78.216             33.033             88.597
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.791269	0.429620	-0.006928
2	6	0	-0.519219	-0.954236	-0.000077
3	6	0	1.686949	-0.536980	-0.005004
4	6	0	0.297184	1.297680	-0.000714
5	6	0	-2.645306	-0.746789	0.003306
6	1	0	-3.708053	-0.954169	0.005446
7	7	0	1.528964	0.817726	-0.000179
8	7	0	0.723431	-1.460380	0.003272
9	7	0	-1.703552	-1.665739	0.006731
10	7	0	-2.171935	0.538674	-0.003861
11	7	0	2.987303	-0.979124	-0.063218
12	1	0	3.703908	-0.325748	0.220051
13	1	0	3.134585	-1.948901	0.181466
14	8	0	0.109136	2.637141	0.007109
15	1	0	0.993558	3.048414	0.003353
16	1	0	-2.716591	1.389408	-0.009911

Guanine: 7H-cis-enol-guanine N2Ha deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.980173872     A.U.
 Zero-point correction=                           0.101297
(Hartree/Particle)
 Thermal correction to Energy=                    0.109868
 Thermal correction to Enthalpy=                  0.110812
 Thermal correction to Gibbs Free Energy=         0.067051
 Sum of electronic and zero-point Energies=           -541.878877
 Sum of electronic and thermal Energies=              -541.870306
```

```
 Sum of electronic and thermal Enthalpies=            -541.869362
 Sum of electronic and thermal Free Energies=         -541.913123

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  68.943             32.229             92.102

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0        0.732698    0.449236    0.002315
    2          6             0        0.515435   -0.951881    0.000620
    3          6             0       -1.770027   -0.692367   -0.000006
    4          6             0       -0.407294    1.247139    0.000239
    5          6             0        2.655252   -0.625319   -0.000458
    6          1             0        3.730012   -0.772076   -0.000565
    7          7             0       -1.604714    0.727690   -0.000079
    8          7             0       -0.666586   -1.539088   -0.000344
    9          7             0        1.769546   -1.595362   -0.000760
   10          7             0        2.116770    0.634317   -0.001112
   11          7             0       -2.978676   -1.200404    0.000165
   12          1             0       -3.631847   -0.412683    0.000190
   13          8             0       -0.288568    2.623480   -0.000833
   14          1             0       -1.213681    2.934326   -0.002235
   15          1             0        2.613305    1.511671    0.007932
 -----------------------------------------------------------------------
```

Guanine: 7H-cis-enol-guanine N2Hb deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.982790335     A.U.
 Zero-point correction=                           0.101619
(Hartree/Particle)
 Thermal correction to Energy=                    0.110051
 Thermal correction to Enthalpy=                  0.110996
 Thermal correction to Gibbs Free Energy=         0.067823
 Sum of electronic and zero-point Energies=           -541.881172
 Sum of electronic and thermal Energies=              -541.872739
 Sum of electronic and thermal Enthalpies=            -541.871795
 Sum of electronic and thermal Free Energies=         -541.914967

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.058             32.044             90.864

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -----------------------------------------------------------------------
    1          6             0        0.741832    0.437048    0.002810
    2          6             0        0.483928   -0.954009    0.000439
    3          6             0       -1.800869   -0.604435   -0.000086
    4          6             0       -0.376777    1.270969    0.000168
```

5	6	0	2.631557	-0.694524	-0.000430
6	1	0	3.701108	-0.874448	-0.000674
7	7	0	-1.588591	0.796660	-0.000750
8	7	0	-0.722932	-1.497393	-0.001124
9	7	0	1.714512	-1.637320	-0.001256
10	7	0	2.130366	0.579525	0.000031
11	7	0	-3.047192	-1.009856	0.001132
12	1	0	-3.013666	-2.033174	0.001240
13	8	0	-0.211666	2.641725	-0.001052
14	1	0	-1.127646	2.980126	-0.002769
15	1	0	2.652365	1.442097	0.006979

Guanine: 7H-cis-enol-guanine N7 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.027306869 A.U.
Zero-point correction= 0.103641
(Hartree/Particle)
Thermal correction to Energy= 0.111472
Thermal correction to Enthalpy= 0.112417
Thermal correction to Gibbs Free Energy= 0.070977
Sum of electronic and zero-point Energies= -541.923666
Sum of electronic and thermal Energies= -541.915834
Sum of electronic and thermal Enthalpies= -541.914890
Sum of electronic and thermal Free Energies= -541.956330

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.950	31.028	87.217

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.860741	0.451865	-0.006647
2	6	0	-0.578189	-0.955227	-0.005821
3	6	0	1.635686	-0.548293	-0.016208
4	6	0	0.249283	1.288167	-0.003790
5	6	0	-2.665445	-0.625254	0.009799
6	1	0	-3.730443	-0.847308	0.017354
7	7	0	1.495733	0.800404	-0.009809
8	7	0	0.682689	-1.467388	-0.007137
9	7	0	-1.749650	-1.635788	0.005212
10	7	0	-2.227856	0.641561	0.003733
11	7	0	2.969941	-1.006952	-0.077702
12	1	0	3.616501	-0.367155	0.370688
13	1	0	3.048955	-1.952193	0.281605
14	8	0	0.140483	2.650958	0.008635
15	1	0	1.061572	2.968589	-0.002803

Guanine: 7H-cis-enol-guanine C8 deprotonated

B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.963421274 A.U.
Zero-point correction= 0.102291
(Hartree/Particle)
Thermal correction to Energy= 0.110542
Thermal correction to Enthalpy= 0.111487
Thermal correction to Gibbs Free Energy= 0.069353
Sum of electronic and zero-point Energies= -541.861130
Sum of electronic and thermal Energies= -541.852879
Sum of electronic and thermal Enthalpies= -541.851935
Sum of electronic and thermal Free Energies= -541.894068

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.366	32.653	88.678

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.849629	0.416480	-0.008575
2	6	0	-0.563958	-0.981324	-0.006109
3	6	0	1.650006	-0.507612	-0.015665
4	6	0	0.219846	1.281794	-0.003643
5	6	0	-2.779847	-0.831508	0.011914
6	7	0	1.484453	0.835244	-0.008527
7	7	0	0.712053	-1.447840	-0.007699
8	7	0	-1.716793	-1.699849	0.006728
9	7	0	-2.232571	0.465074	0.003516
10	7	0	2.987623	-0.945983	-0.076492
11	1	0	3.630877	-0.298371	0.364474
12	1	0	3.082407	-1.893082	0.273199
13	8	0	0.052449	2.645933	0.008908
14	1	0	0.957319	3.006664	-0.002706
15	1	0	-2.792063	1.303814	0.003555

Guanine: 7H-cis-enol-guanine OH deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.033154424 A.U.
Zero-point correction= 0.103459
(Hartree/Particle)
Thermal correction to Energy= 0.111428
Thermal correction to Enthalpy= 0.112372
Thermal correction to Gibbs Free Energy= 0.070620
Sum of electronic and zero-point Energies= -541.929695
Sum of electronic and thermal Energies= -541.921726
Sum of electronic and thermal Enthalpies= -541.920782
Sum of electronic and thermal Free Energies= -541.962534

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	69.922	31.351	87.875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.767415	0.420494	-0.011576
2	6	0	-0.478861	-0.942036	-0.006145
3	6	0	1.695096	-0.435976	-0.016993
4	6	0	0.260967	1.429890	-0.002986
5	6	0	-2.618331	-0.774330	0.010425
6	1	0	-3.679082	-0.996230	0.018297
7	7	0	1.531876	0.899515	-0.007395
8	7	0	0.789671	-1.424885	-0.008130
9	7	0	-1.656841	-1.682085	0.007172
10	7	0	-2.148691	0.509395	0.000225
11	7	0	3.039923	-0.859936	-0.075858
12	1	0	3.669311	-0.166203	0.311648
13	1	0	3.165938	-1.783817	0.322586
14	8	0	0.009566	2.661430	0.012232
15	1	0	-2.673001	1.372534	0.001159

Guanine: 7H-cis-enol-guanine OHb protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.837614161 A.U.
Zero-point correction= 0.126356
(Hartree/Particle)
Thermal correction to Energy= 0.135703
Thermal correction to Enthalpy= 0.136648
Thermal correction to Gibbs Free Energy= 0.092190
Sum of electronic and zero-point Energies= -542.717623
Sum of electronic and thermal Energies= -542.708275
Sum of electronic and thermal Enthalpies= -542.707331
Sum of electronic and thermal Free Energies= -542.751789

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.155	36.095	93.569

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.828165	0.444212	0.001226
2	6	0	0.554011	-0.977997	0.000032
3	6	0	-1.684879	-0.639899	-0.000372
4	6	0	-0.326403	1.170603	0.000003
5	6	0	2.678164	-0.748396	-0.000182
6	1	0	3.742414	-0.950090	-0.000094
7	7	0	-1.535714	0.725285	-0.000138
8	7	0	-0.660391	-1.504132	-0.000586
9	7	0	1.743979	-1.663780	-0.000452
10	7	0	2.207557	0.547866	-0.000197

11	7	0	-2.940286	-1.120472	0.000359
12	1	0	-3.738175	-0.502206	0.001453
13	1	0	-3.084303	-2.121211	0.001640
14	8	0	-0.356459	2.681439	-0.000913
15	1	0	-1.262693	3.067705	0.002767
16	1	0	2.787197	1.376390	0.006159
17	1	0	0.406880	3.293392	-0.001753

Guanine: 7H-cis-enol-guanine N1 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.917285926 A.U.
Zero-point correction= 0.127655
(Hartree/Particle)
Thermal correction to Energy= 0.136944
Thermal correction to Enthalpy= 0.137888
Thermal correction to Gibbs Free Energy= 0.093470
Sum of electronic and zero-point Energies= -542.789632
Sum of electronic and thermal Energies= -542.780344
Sum of electronic and thermal Enthalpies= -542.779399
Sum of electronic and thermal Free Energies= -542.823817

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.933	35.605	93.486

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.827620	0.419715	0.000732
2	6	0	-0.518351	-0.975880	-0.002666
3	6	0	1.702229	-0.577691	0.003208
4	6	0	0.196013	1.330924	0.000219
5	6	0	-2.638081	-0.809655	0.000844
6	1	0	-3.693698	-1.052215	0.000512
7	7	0	1.463848	0.801889	-0.002212
8	7	0	0.730625	-1.462555	0.004639
9	7	0	-1.666452	-1.704985	-0.002632
10	7	0	-2.207086	0.486559	0.004658
11	7	0	2.988156	-0.979693	-0.023119
12	1	0	3.774639	-0.367950	0.144758
13	1	0	3.155235	-1.978169	0.021688
14	8	0	-0.017353	2.642215	-0.004621
15	1	0	0.781902	3.196670	0.036458
16	1	0	-2.785893	1.318062	0.005975
17	1	0	2.257862	1.432896	-0.055792

Guanine: 7H-cis-enol-guanine N2 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.914049450   A.U.
 Zero-point correction=   0.130898
(Hartree/Particle)
 Thermal correction to Energy=   0.139347
 Thermal correction to Enthalpy=   0.140291
 Thermal correction to Gibbs Free Energy=   0.097361
 Sum of electronic and zero-point Energies=   -542.783152
 Sum of electronic and thermal Energies=   -542.774703
 Sum of electronic and thermal Enthalpies=   -542.773758
 Sum of electronic and thermal Free Energies=   -542.816688

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.442	32.750	90.354

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.846577	0.411129	-0.000288
2	6	0	0.535379	-0.970367	-0.000169
3	6	0	-1.600761	-0.429717	-0.000093
4	6	0	-0.196892	1.341339	-0.000140
5	6	0	2.649125	-0.840446	0.000169
6	1	0	3.702981	-1.088205	0.000392
7	7	0	-1.459831	0.891541	-0.000058
8	7	0	-0.746965	-1.413816	-0.000160
9	7	0	1.669418	-1.723764	0.000067
10	7	0	2.219012	0.462265	0.000201
11	7	0	-3.032055	-0.878301	0.000162
12	1	0	-3.534030	-0.531898	-0.828081
13	1	0	-3.048003	-1.907645	-0.000853
14	8	0	0.055411	2.647364	0.000125
15	1	0	-0.779452	3.153332	0.000325
16	1	0	2.800702	1.292108	-0.000864
17	1	0	-3.533110	-0.533707	0.829731

Guanine: 7H-cis-enol-guanine N3 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.945430790   A.U.
 Zero-point correction=   0.129744
(Hartree/Particle)
 Thermal correction to Energy=   0.138214
 Thermal correction to Enthalpy=   0.139158
 Thermal correction to Gibbs Free Energy=   0.096600
 Sum of electronic and zero-point Energies=   -542.815687
 Sum of electronic and thermal Energies=   -542.807217
 Sum of electronic and thermal Enthalpies=   -542.806273
 Sum of electronic and thermal Free Energies=   -542.848831

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	86.730	34.003	89.571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.822063	0.442704	-0.000774
2	6	0	0.570208	-0.927533	-0.000371
3	6	0	-1.742618	-0.465023	0.000009
4	6	0	-0.270084	1.325903	-0.000191
5	6	0	2.667382	-0.748829	0.000427
6	1	0	3.724792	-0.978604	0.000886
7	7	0	-1.513750	0.853815	0.000087
8	7	0	-0.725499	-1.380621	-0.000748
9	7	0	1.698651	-1.662143	0.000266
10	7	0	2.202504	0.529289	0.000114
11	7	0	-3.012085	-0.893488	0.000626
12	1	0	-3.751680	-0.202189	-0.000542
13	1	0	-3.272165	-1.870537	-0.000405
14	8	0	-0.060080	2.632217	0.000187
15	1	0	-0.913952	3.109061	0.000695
16	1	0	2.759351	1.376396	-0.000472
17	1	0	-0.896151	-2.383158	0.001328

Guanine: 7H-cis-enol-guanine N7H protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.873518849 A.U.
Zero-point correction= 0.128941
(Hartree/Particle)
Thermal correction to Energy= 0.137384
Thermal correction to Enthalpy= 0.138328
Thermal correction to Gibbs Free Energy= 0.095694
Sum of electronic and zero-point Energies= -542.744578
Sum of electronic and thermal Energies= -542.736135
Sum of electronic and thermal Enthalpies= -542.735191
Sum of electronic and thermal Free Energies= -542.777825

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.210	33.764	89.731

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.734008	0.425746	0.001119
2	6	0	0.453616	-0.940043	0.000324
3	6	0	-1.741881	-0.527040	0.000010
4	6	0	-0.346540	1.309407	0.000083
5	6	0	2.633312	-0.889276	-0.000491
6	1	0	3.699923	-1.084372	-0.000811
7	7	0	-1.574259	0.822052	-0.000142

8	7	0	-0.743321	-1.462377	-0.000064
9	7	0	1.669620	-1.696508	-0.000302
10	7	0	2.182536	0.594159	0.000223
11	7	0	-2.996100	-0.990014	-0.000120
12	1	0	-3.778748	-0.350010	0.000303
13	1	0	-3.163951	-1.987518	0.000262
14	8	0	-0.129193	2.625577	-0.000313
15	1	0	-0.987208	3.094607	-0.000947
16	1	0	2.550152	1.089071	0.828421
17	1	0	2.548951	1.089658	-0.828159

Guanine: 7H-cis-enol-guanine N9 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.943236443 A.U.
Zero-point correction= 0.130075
(Hartree/Particle)
Thermal correction to Energy= 0.138370
Thermal correction to Enthalpy= 0.139314
Thermal correction to Gibbs Free Energy= 0.097105
Sum of electronic and zero-point Energies= -542.813162
Sum of electronic and thermal Energies= -542.804867
Sum of electronic and thermal Enthalpies= -542.803922
Sum of electronic and thermal Free Energies= -542.846131

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.828	33.654	88.836

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.752507	0.467551	-0.000900
2	6	0	-0.475234	-0.901644	-0.000373
3	6	0	1.718728	-0.560193	0.000051
4	6	0	0.369299	1.323091	-0.000230
5	6	0	-2.692344	-0.603056	0.000460
6	1	0	-3.753681	-0.805762	0.000838
7	7	0	1.573932	0.800478	0.000169
8	7	0	0.713946	-1.469019	-0.000034
9	7	0	-1.720029	-1.533091	0.000324
10	7	0	-2.135732	0.607489	-0.000246
11	7	0	2.976844	-1.022916	0.000159
12	1	0	3.755597	-0.379006	-0.000217
13	1	0	3.150661	-2.018648	-0.000484
14	8	0	0.180603	2.641397	0.000337
15	1	0	1.048100	3.092240	0.000979
16	1	0	-2.649911	1.483067	-0.000791
17	1	0	-1.865975	-2.538137	0.000328

Guanine: NEUTRAL 1H9H-keto-guanine
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.545110294     A.U.
 Zero-point correction=                           0.115805
(Hartree/Particle)
 Thermal correction to Energy=                    0.124350
 Thermal correction to Enthalpy=                  0.125295
 Thermal correction to Gibbs Free Energy=         0.082401
 Sum of electronic and zero-point Energies=           -542.429305
 Sum of electronic and thermal Energies=              -542.420760
 Sum of electronic and thermal Enthalpies=            -542.419816
 Sum of electronic and thermal Free Energies=         -542.462709

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  78.031             33.509             90.277
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.836318	0.502059	0.006560
2	6	0	-0.551170	-0.845822	-0.010008
3	6	0	1.740864	-0.388891	0.011031
4	6	0	0.261247	1.476527	-0.001226
5	6	0	-2.721836	-0.512821	0.008572
6	1	0	-3.775107	-0.759148	0.004106
7	7	0	1.554102	0.888539	0.041305
8	7	0	0.730951	-1.355091	0.017095
9	7	0	-1.747462	-1.508272	-0.004040
10	7	0	-2.208835	0.687240	0.016268
11	7	0	3.020124	-0.917127	-0.074568
12	1	0	3.727000	-0.195207	0.016515
13	1	0	3.213879	-1.728140	0.503726
14	8	0	0.125353	2.688223	-0.029069
15	1	0	-1.905195	-2.506775	0.012599
16	1	0	0.937710	-2.269853	-0.366383

Guanine: 1H9H-keto-guanine N2Ha deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.995945990     A.U.
 Zero-point correction=                           0.101743
(Hartree/Particle)
 Thermal correction to Energy=                    0.110135
 Thermal correction to Enthalpy=                  0.111079
 Thermal correction to Gibbs Free Energy=         0.068228
 Sum of electronic and zero-point Energies=           -541.894204
 Sum of electronic and thermal Energies=              -541.885812
 Sum of electronic and thermal Enthalpies=            -541.884867
 Sum of electronic and thermal Free Energies=         -541.927719

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
```

```
 Total                  69.111             32.286             90.188
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.769190    0.515773   -0.016663
    2          6             0       -0.533410   -0.842167    0.026645
    3          6             0        1.828654   -0.495198    0.008904
    4          6             0        0.392804    1.440822    0.016124
    5          6             0       -2.702618   -0.430979   -0.044530
    6          1             0       -3.763899   -0.640038   -0.085952
    7          7             0        1.628582    0.842622    0.026011
    8          7             0        0.709741   -1.388212    0.143067
    9          7             0       -1.759865   -1.460478    0.011955
   10          7             0       -2.137959    0.749215   -0.062905
   11          7             0        2.971333   -1.125159   -0.103520
   12          1             0        3.697772   -0.411660   -0.181610
   13          8             0        0.239986    2.675036    0.030626
   14          1             0       -1.945210   -2.451687    0.065781
   15          1             0        0.911175   -2.352330   -0.088353
 -------------------------------------------------------------------
```

Guanine: 1H9H-keto-guanine N2Hb deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.980871662     A.U.
 Zero-point correction=                           0.100957
(Hartree/Particle)
 Thermal correction to Energy=                    0.109420
 Thermal correction to Enthalpy=                  0.110364
 Thermal correction to Gibbs Free Energy=         0.067388
 Sum of electronic and zero-point Energies=           -541.879914
 Sum of electronic and thermal Energies=              -541.871452
 Sum of electronic and thermal Enthalpies=            -541.870508
 Sum of electronic and thermal Free Energies=         -541.913484

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  68.662             32.615             90.451

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.781348    0.504850    0.011165
    2          6             0        0.511737   -0.843316   -0.022815
    3          6             0       -1.865549   -0.423587   -0.004403
    4          6             0       -0.359995    1.457204   -0.010947
    5          6             0        2.690761   -0.488129    0.036509
    6          1             0        3.746845   -0.722419    0.079015
    7          7             0       -1.608145    0.895314   -0.021968
    8          7             0       -0.748450   -1.371651   -0.142941
    9          7             0        1.723783   -1.493142   -0.008972
   10          7             0        2.155772    0.706069    0.051330
```

11	7	0	-3.074251	-0.920063	0.099281
12	1	0	-3.038147	-1.942565	0.037165
13	8	0	-0.170259	2.686057	-0.020372
14	1	0	1.885179	-2.487160	-0.085738
15	1	0	-0.922592	-2.294137	0.238371

Guanine: 1H9H-keto-guanine N3 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.028432690 A.U.
Zero-point correction= 0.103097
(Hartree/Particle)
Thermal correction to Energy= 0.111148
Thermal correction to Enthalpy= 0.112092
Thermal correction to Gibbs Free Energy= 0.070166
Sum of electronic and zero-point Energies= -541.925335
Sum of electronic and thermal Energies= -541.917284
Sum of electronic and thermal Enthalpies= -541.916340
Sum of electronic and thermal Free Energies= -541.958267

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.747	31.634	88.242

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.807661	0.503372	-0.005255
2	6	0	-0.496840	-0.857868	-0.004366
3	6	0	1.676442	-0.477780	-0.017322
4	6	0	0.299872	1.454399	-0.002555
5	6	0	-2.693202	-0.523120	0.007511
6	1	0	-3.748515	-0.769024	0.012930
7	7	0	1.557610	0.846396	-0.007750
8	7	0	0.719906	-1.433651	-0.009004
9	7	0	-1.716255	-1.509198	0.004863
10	7	0	-2.187957	0.685722	0.003217
11	7	0	2.996403	-0.970545	-0.075533
12	1	0	3.660677	-0.294206	0.283259
13	1	0	3.087355	-1.886930	0.348734
14	8	0	0.173214	2.691965	0.009879
15	1	0	-1.844843	-2.510644	-0.002586

Guanine: 1H9H-keto-guanine C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.938377697 A.U.
Zero-point correction= 0.101294
(Hartree/Particle)

```
 Thermal correction to Energy=                    0.109942
 Thermal correction to Enthalpy=                  0.110886
 Thermal correction to Gibbs Free Energy=         0.067792
 Sum of electronic and zero-point Energies=           -541.837084
 Sum of electronic and thermal Energies=              -541.828436
 Sum of electronic and thermal Enthalpies=            -541.827491
 Sum of electronic and thermal Free Energies=         -541.870586

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  68.990             33.457            90.700

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.901682    0.477464    0.013705
    2          6             0       -0.579971   -0.869188   -0.009775
    3          6             0        1.708556   -0.365289    0.000719
    4          6             0        0.168756    1.460743   -0.001303
    5          6             0       -2.863730   -0.598552    0.010414
    6          7             0        1.497860    0.907117    0.037926
    7          7             0        0.729000   -1.336026    0.006965
    8          7             0       -1.757656   -1.545743   -0.006753
    9          7             0       -2.287147    0.613993    0.023969
   10          7             0        3.026012   -0.877341   -0.077775
   11          1             0        3.674924   -0.097949   -0.014767
   12          1             0        3.231153   -1.555846    0.652859
   13          8             0        0.046236    2.686417   -0.031261
   14          1             0       -1.883633   -2.547823   -0.010751
   15          1             0        0.959617   -2.254784   -0.350132
 -------------------------------------------------------------------
```

Guanine: 1H9H-keto-guanine N9 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.021616409     A.U.
 Zero-point correction=                           0.103209
(Hartree/Particle)
 Thermal correction to Energy=                    0.111348
 Thermal correction to Enthalpy=                  0.112292
 Thermal correction to Gibbs Free Energy=         0.070073
 Sum of electronic and zero-point Energies=           -541.918408
 Sum of electronic and thermal Energies=              -541.910269
 Sum of electronic and thermal Enthalpies=            -541.909325
 Sum of electronic and thermal Free Energies=         -541.951544

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.872             31.526            88.857

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.881736	0.480451	0.022290
2	6	0	-0.594945	-0.891375	0.004285
3	6	0	1.700047	-0.384901	-0.008336
4	6	0	0.185197	1.460439	0.001174
5	6	0	-2.670468	-0.663471	-0.000127
6	1	0	-3.724496	-0.927277	-0.007766
7	7	0	1.503342	0.896790	0.021243
8	7	0	0.722555	-1.340815	0.000285
9	7	0	-1.706024	-1.643373	-0.010287
10	7	0	-2.258793	0.606630	0.019547
11	7	0	3.021135	-0.889134	-0.081122
12	1	0	3.665192	-0.110667	0.025308
13	1	0	3.214886	-1.599633	0.621122
14	8	0	0.064063	2.690499	-0.021159
15	1	0	0.927839	-2.303958	-0.232768

Guanine: 1H9H-keto-guanine OHa protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.930644660 A.U.
Zero-point correction= 0.129081
(Hartree/Particle)
Thermal correction to Energy= 0.137722
Thermal correction to Enthalpy= 0.138666
Thermal correction to Gibbs Free Energy= 0.095785
Sum of electronic and zero-point Energies= -542.801563
Sum of electronic and thermal Energies= -542.792923
Sum of electronic and thermal Enthalpies= -542.791979
Sum of electronic and thermal Free Energies= -542.834860

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.422	34.508	90.250

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.837405	0.479529	0.000008
2	6	0	-0.578162	-0.888229	-0.000016
3	6	0	1.733585	-0.484809	-0.000007
4	6	0	0.291494	1.332586	-0.000024
5	6	0	-2.735778	-0.476594	-0.000048
6	1	0	-3.794808	-0.697878	-0.000074
7	7	0	1.529961	0.828897	0.000005
8	7	0	0.695460	-1.392300	0.000089
9	7	0	-1.784443	-1.505668	0.000061
10	7	0	-2.197662	0.708756	-0.000019
11	7	0	2.992172	-0.947321	-0.000166
12	1	0	3.746343	-0.271478	0.000347
13	1	0	3.233750	-1.928821	0.000497
14	8	0	0.128993	2.635696	0.000030

15	1	0	-1.982560	-2.499779	0.000068
16	1	0	0.875486	-2.391385	-0.000374
17	1	0	0.999023	3.082319	0.000018

Guanine: 1H9H-keto-guanine OHb protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.929918198     A.U.
 Zero-point correction=                           0.129183
(Hartree/Particle)
 Thermal correction to Energy=                    0.137807
 Thermal correction to Enthalpy=                  0.138751
 Thermal correction to Gibbs Free Energy=         0.095897
 Sum of electronic and zero-point Energies=           -542.800735
 Sum of electronic and thermal Energies=              -542.792111
 Sum of electronic and thermal Enthalpies=            -542.791167
 Sum of electronic and thermal Free Energies=         -542.834021

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.475             34.439            90.194
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.824974	0.437972	0.000034
2	6	0	-0.532803	-0.918092	-0.000025
3	6	0	1.760363	-0.420707	0.000093
4	6	0	0.266099	1.340366	0.000003
5	6	0	-2.703231	-0.556180	-0.000025
6	1	0	-3.757119	-0.800258	-0.000073
7	7	0	1.516341	0.884574	0.000058
8	7	0	0.756987	-1.374754	0.000144
9	7	0	-1.729005	-1.560388	-0.000019
10	7	0	-2.188317	0.642199	0.000054
11	7	0	3.034387	-0.836482	-0.000320
12	1	0	3.759114	-0.128317	0.000411
13	1	0	3.315463	-1.807395	0.001124
14	8	0	0.114982	2.647898	-0.000055
15	1	0	-1.907186	-2.558416	0.000001
16	1	0	0.976666	-2.365822	-0.000849
17	1	0	-0.832270	2.890824	-0.000076

Guanine: 1H9H-keto-guanine N1 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.921133662     A.U.
 Zero-point correction=                           0.128412
(Hartree/Particle)
 Thermal correction to Energy=                    0.137488
```

```
 Thermal correction to Enthalpy=                  0.138432
 Thermal correction to Gibbs Free Energy=         0.094589
 Sum of electronic and zero-point Energies=           -542.792722
 Sum of electronic and thermal Energies=              -542.783646
 Sum of electronic and thermal Enthalpies=            -542.782702
 Sum of electronic and thermal Free Energies=         -542.826544

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.275             35.400             92.275

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.890962    0.506144   -0.000313
    2          6             0       -0.579537   -0.841212   -0.000005
    3          6             0        1.752287   -0.482790    0.000036
    4          6             0        0.158854    1.497822   -0.000006
    5          6             0       -2.750540   -0.530568    0.000118
    6          1             0       -3.800433   -0.790910    0.000230
    7          7             0        1.481205    0.830332    0.000041
    8          7             0        0.712637   -1.352327   -0.000179
    9          7             0       -1.761610   -1.512771    0.000221
   10          7             0       -2.254725    0.676467   -0.000257
   11          7             0        3.011619   -0.940071   -0.000125
   12          1             0        3.800961   -0.306021   -0.000715
   13          1             0        3.228225   -1.928815    0.001323
   14          8             0        0.135784    2.698260    0.000145
   15          1             0       -1.917621   -2.514374    0.000612
   16          1             0        0.887883   -2.350686   -0.000631
   17          1             0        2.250227    1.496937    0.001134
 -------------------------------------------------------------------
```

Guanine: 1H9H-keto-guanine N2 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.859122254     A.U.
 Zero-point correction=                           0.128595
(Hartree/Particle)
 Thermal correction to Energy=                    0.137835
 Thermal correction to Enthalpy=                  0.138779
 Thermal correction to Gibbs Free Energy=         0.094153
 Sum of electronic and zero-point Energies=           -542.730527
 Sum of electronic and thermal Energies=              -542.721287
 Sum of electronic and thermal Enthalpies=            -542.720343
 Sum of electronic and thermal Free Energies=         -542.764970

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.493             34.641             93.924

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	-0.898927	0.490180	0.000094
2	6	0	-0.585606	-0.860335	-0.000023
3	6	0	1.648328	-0.341035	-0.000084
4	6	0	0.145333	1.510686	0.000002
5	6	0	-2.755770	-0.563704	0.000090
6	1	0	-3.804582	-0.828881	0.000111
7	7	0	1.487127	0.911329	0.000149
8	7	0	0.718918	-1.342357	-0.000156
9	7	0	-1.764568	-1.541894	-0.000122
10	7	0	-2.265369	0.645978	0.000160
11	7	0	3.092034	-0.789021	0.000145
12	1	0	3.631046	0.092397	-0.000953
13	1	0	3.359648	-1.325940	0.837845
14	8	0	0.029526	2.707948	-0.000225
15	1	0	-1.915761	-2.543599	0.000394
16	1	0	0.936765	-2.332476	-0.001072
17	1	0	3.359527	-1.328074	-0.836217

Guanine: 1H9H-keto-guanine N3H protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.838257982 A.U.
Zero-point correction= 0.127577
(Hartree/Particle)
Thermal correction to Energy= 0.136799
Thermal correction to Enthalpy= 0.137743
Thermal correction to Gibbs Free Energy= 0.093071
Sum of electronic and zero-point Energies= -542.710681
Sum of electronic and thermal Energies= -542.701459
Sum of electronic and thermal Enthalpies= -542.700515
Sum of electronic and thermal Free Energies= -542.745187

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.843	35.184	94.020

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.855245	0.495857	-0.006536
2	6	0	-0.591172	-0.850310	-0.001132
3	6	0	1.848023	-0.255229	0.029717
4	6	0	0.207591	1.516490	0.006265
5	6	0	-2.745177	-0.501044	-0.008018
6	1	0	-3.803934	-0.724281	-0.013146
7	7	0	1.532644	0.949276	0.048436
8	7	0	0.727826	-1.447108	0.013153
9	7	0	-1.795081	-1.503773	0.001594
10	7	0	-2.210751	0.696023	-0.011717
11	7	0	3.067266	-0.818155	-0.082000

12	1	0	3.851253	-0.171070	-0.082023
13	1	0	3.274631	-1.756457	0.238782
14	8	0	0.054482	2.706456	-0.007847
15	1	0	-1.981702	-2.500706	-0.005793
16	1	0	0.913356	-2.021355	-0.822560
17	1	0	0.873090	-2.046205	0.839471

Guanine: 1H9H-keto-guanine N7 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.914895265 A.U.
Zero-point correction= 0.128944
(Hartree/Particle)
Thermal correction to Energy= 0.137824
Thermal correction to Enthalpy= 0.138768
Thermal correction to Gibbs Free Energy= 0.095224
Sum of electronic and zero-point Energies= -542.785951
Sum of electronic and thermal Energies= -542.777072
Sum of electronic and thermal Enthalpies= -542.776128
Sum of electronic and thermal Free Energies= -542.819671

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.486	34.747	91.645

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.764005	0.462385	0.004653
2	6	0	-0.499710	-0.880255	-0.005435
3	6	0	1.793226	-0.366798	0.008949
4	6	0	0.305659	1.475377	-0.002634
5	6	0	-2.703957	-0.614581	0.002939
6	1	0	-3.761567	-0.833483	0.000065
7	7	0	1.575512	0.916993	0.020781
8	7	0	0.779631	-1.355468	0.013111
9	7	0	-1.712545	-1.540171	-0.002510
10	7	0	-2.138883	0.588652	0.009553
11	7	0	3.056415	-0.844664	-0.038579
12	1	0	3.795330	-0.153294	0.018320
13	1	0	3.292613	-1.789402	0.234050
14	8	0	0.058303	2.667968	-0.016660
15	1	0	-1.872761	-2.542631	-0.001057
16	1	0	0.997920	-2.322027	-0.199284
17	1	0	-2.626154	1.482932	0.013862

Guanine: 1H9H-keto-guanine N9H protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.824606532   A.U.
 Zero-point correction=   0.126900
(Hartree/Particle)
 Thermal correction to Energy=   0.135955
 Thermal correction to Enthalpy=   0.136899
 Thermal correction to Gibbs Free Energy=   0.092896
 Sum of electronic and zero-point Energies=   -542.697707
 Sum of electronic and thermal Energies=   -542.688652
 Sum of electronic and thermal Enthalpies=   -542.687708
 Sum of electronic and thermal Free Energies=   -542.731710

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.313	35.437	92.612

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.775918	0.519749	0.011934
2	6	0	0.511703	-0.803892	0.058216
3	6	0	-1.790342	-0.396308	-0.023857
4	6	0	-0.349215	1.494849	0.012839
5	6	0	2.787901	-0.322831	-0.047555
6	1	0	3.845479	-0.556656	-0.055402
7	7	0	-1.608235	0.882034	-0.053911
8	7	0	-0.731652	-1.356647	0.013955
9	7	0	1.787004	-1.533316	0.006591
10	7	0	2.165612	0.768352	-0.041157
11	7	0	-3.031523	-0.939789	0.019553
12	1	0	-3.795721	-0.276855	-0.054206
13	1	0	-3.214853	-1.867114	-0.342845
14	8	0	-0.182174	2.692453	0.048485
15	1	0	1.880897	-2.126290	-0.832686
16	1	0	-0.921623	-2.284259	0.380948
17	1	0	1.978986	-2.122297	0.831631

Guanine: NEUTRAL 1H7H-keto-guanine
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.566882870   A.U.
 Zero-point correction=   0.116615
(Hartree/Particle)
 Thermal correction to Energy=   0.125007
 Thermal correction to Enthalpy=   0.125951
 Thermal correction to Gibbs Free Energy=   0.083366
 Sum of electronic and zero-point Energies=   -542.450268
 Sum of electronic and thermal Energies=   -542.441876
 Sum of electronic and thermal Enthalpies=   -542.440932
 Sum of electronic and thermal Free Energies=   -542.483517

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.443	33.000	89.628

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.806105	0.442288	0.016450
2	6	0	-0.539167	-0.908378	0.005173
3	6	0	1.748647	-0.361731	0.000294
4	6	0	0.231771	1.458127	0.000474
5	6	0	-2.647030	-0.769712	-0.003936
6	1	0	-3.701465	-1.009071	-0.010871
7	7	0	1.528006	0.924575	0.016925
8	7	0	0.772545	-1.338197	0.006971
9	7	0	-1.667083	-1.669148	-0.006800
10	7	0	-2.185752	0.510765	0.010852
11	1	0	-2.726683	1.365901	0.014770
12	7	0	3.048375	-0.824446	-0.073508
13	1	0	3.728157	-0.085923	0.066686
14	1	0	3.270955	-1.679826	0.422182
15	8	0	0.005045	2.666640	-0.015017
16	1	0	0.987349	-2.312607	-0.164442

Guanine: 1H7H-keto-guanine N2Ha deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -541.995945990     A.U.
 Zero-point correction=                           0.101743
(Hartree/Particle)
 Thermal correction to Energy=                    0.110135
 Thermal correction to Enthalpy=                  0.111079
 Thermal correction to Gibbs Free Energy=         0.068228
 Sum of electronic and zero-point Energies=           -541.894204
 Sum of electronic and thermal Energies=              -541.885812
 Sum of electronic and thermal Enthalpies=            -541.884867
 Sum of electronic and thermal Free Energies=         -541.927719

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.111             32.286             90.188
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.769190	0.515773	-0.016663
2	6	0	-0.533410	-0.842167	0.026645
3	6	0	1.828654	-0.495198	0.008904
4	6	0	0.392804	1.440822	0.016124
5	6	0	-2.702618	-0.430979	-0.044530
6	1	0	-3.763899	-0.640038	-0.085952
7	7	0	1.628582	0.842622	0.026011
8	7	0	0.709741	-1.388212	0.143067
9	7	0	-1.759865	-1.460478	0.011955

10	7	0	-2.137959	0.749215	-0.062905
11	7	0	2.971333	-1.125159	-0.103520
12	1	0	3.697772	-0.411660	-0.181610
13	8	0	0.239986	2.675036	0.030626
14	1	0	-1.945210	-2.451687	0.065781
15	1	0	0.911175	-2.352330	-0.088353

Guanine: 1H7H-keto-guanine N2Hb deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.995945990 A.U.
Zero-point correction= 0.101743
(Hartree/Particle)
Thermal correction to Energy= 0.110135
Thermal correction to Enthalpy= 0.111079
Thermal correction to Gibbs Free Energy= 0.068228
Sum of electronic and zero-point Energies= -541.894204
Sum of electronic and thermal Energies= -541.885812
Sum of electronic and thermal Enthalpies= -541.884867
Sum of electronic and thermal Free Energies= -541.927719

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.111	32.286	90.188

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.769190	0.515773	-0.016663
2	6	0	-0.533410	-0.842167	0.026645
3	6	0	1.828654	-0.495198	0.008904
4	6	0	0.392804	1.440822	0.016124
5	6	0	-2.702618	-0.430979	-0.044530
6	1	0	-3.763899	-0.640038	-0.085952
7	7	0	1.628582	0.842622	0.026011
8	7	0	0.709741	-1.388212	0.143067
9	7	0	-1.759865	-1.460478	0.011955
10	7	0	-2.137959	0.749215	-0.062905
11	7	0	2.971333	-1.125159	-0.103520
12	1	0	3.697772	-0.411660	-0.181610
13	8	0	0.239986	2.675036	0.030626
14	1	0	-1.945210	-2.451687	0.065781
15	1	0	0.911175	-2.352330	-0.088353

Guanine: 1H7H-keto-guanine N3 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.033154373 A.U.

```
 Zero-point correction=                           0.103458
(Hartree/Particle)
 Thermal correction to Energy=                    0.111428
 Thermal correction to Enthalpy=                  0.112372
 Thermal correction to Gibbs Free Energy=         0.070617
 Sum of electronic and zero-point Energies=           -541.929697
 Sum of electronic and thermal Energies=              -541.921727
 Sum of electronic and thermal Enthalpies=            -541.920783
 Sum of electronic and thermal Free Energies=         -541.962537

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.922             31.355             87.880
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.767370	0.420357	-0.010559
2	6	0	-0.479053	-0.942041	-0.005758
3	6	0	1.695067	-0.436229	-0.017046
4	6	0	0.261398	1.430064	-0.003145
5	6	0	-2.618456	-0.774154	0.009990
6	1	0	-3.679278	-0.995642	0.017337
7	7	0	1.531874	0.899334	-0.007652
8	7	0	0.789584	-1.424956	-0.008028
9	7	0	-1.657033	-1.682052	0.006699
10	7	0	-2.148485	0.509582	0.000449
11	1	0	-2.672670	1.372799	0.003044
12	7	0	3.039714	-0.860062	-0.075856
13	1	0	3.668984	-0.166324	0.311830
14	1	0	3.165743	-1.783829	0.322810
15	8	0	0.009767	2.661512	0.011850

Guanine: 1H7H-keto-guanine N7 deprotonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.021616323     A.U.
 Zero-point correction=                           0.103209
(Hartree/Particle)
 Thermal correction to Energy=                    0.111348
 Thermal correction to Enthalpy=                  0.112292
 Thermal correction to Gibbs Free Energy=         0.070073
 Sum of electronic and zero-point Energies=           -541.918408
 Sum of electronic and thermal Energies=              -541.910269
 Sum of electronic and thermal Enthalpies=            -541.909325
 Sum of electronic and thermal Free Energies=         -541.951544

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  69.872             31.526             88.857
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.881761	0.480553	0.021985
2	6	0	-0.595031	-0.891261	0.003911
3	6	0	1.699996	-0.385169	-0.008602
4	6	0	0.185408	1.460416	0.001096
5	6	0	-2.670562	-0.663349	0.000250
6	1	0	-3.724634	-0.927056	-0.007025
7	7	0	1.503434	0.896647	0.020803
8	7	0	0.722354	-1.340667	-0.000955
9	7	0	-1.706213	-1.643267	-0.009886
10	7	0	-2.258789	0.606751	0.019389
11	7	0	3.021215	-0.889280	-0.080584
12	1	0	3.664963	-0.110675	0.026809
13	1	0	3.214623	-1.599970	0.621580
14	8	0	0.064404	2.690531	-0.020686
15	1	0	0.927507	-2.304988	-0.229081

Guanine: 1H7H-keto-guanine C8 deprotonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -541.965784421 A.U.
Zero-point correction= 0.102673
(Hartree/Particle)
Thermal correction to Energy= 0.111024
Thermal correction to Enthalpy= 0.111969
Thermal correction to Gibbs Free Energy= 0.069436
Sum of electronic and zero-point Energies= -541.863112
Sum of electronic and thermal Energies= -541.854760
Sum of electronic and thermal Enthalpies= -541.853816
Sum of electronic and thermal Free Energies= -541.896349

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.669	32.493	89.518

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.862222	0.431705	0.024128
2	6	0	-0.577234	-0.925891	0.004566
3	6	0	1.710428	-0.340047	-0.009229
4	6	0	0.146680	1.446215	-0.000217
5	6	0	-2.772909	-0.864942	-0.002627
6	7	0	1.478998	0.938700	0.015609
7	7	0	0.755555	-1.320305	-0.004836
8	7	0	-1.669287	-1.710913	-0.011648
9	7	0	-2.253383	0.426697	0.017344
10	1	0	-2.822864	1.259368	0.028003
11	7	0	3.042188	-0.805111	-0.078277

12	1	0	3.669322	-0.015783	0.044598
13	1	0	3.251922	-1.531880	0.601680
14	8	0	-0.053776	2.673871	-0.018677
15	1	0	0.984878	-2.288389	-0.191938

Guanine: 1H7H-keto-guanine OHa protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.945430978     A.U.
 Zero-point correction=                           0.129745
(Hartree/Particle)
 Thermal correction to Energy=                    0.138214
 Thermal correction to Enthalpy=                  0.139159
 Thermal correction to Gibbs Free Energy=         0.096600
 Sum of electronic and zero-point Energies=           -542.815686
 Sum of electronic and thermal Energies=              -542.807217
 Sum of electronic and thermal Enthalpies=            -542.806272
 Sum of electronic and thermal Free Energies=         -542.848831

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.731             34.003             89.571
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.821925	0.442711	-0.000117
2	6	0	-0.570148	-0.927640	-0.000059
3	6	0	1.742569	-0.464910	-0.000084
4	6	0	0.270011	1.325910	-0.000067
5	6	0	-2.667464	-0.748684	0.000017
6	1	0	-3.724839	-0.978653	0.000076
7	7	0	1.513745	0.853833	-0.000017
8	7	0	0.725495	-1.380684	-0.000276
9	7	0	-1.698664	-1.662108	0.000170
10	7	0	-2.202494	0.529222	-0.000008
11	1	0	-2.759368	1.376308	0.000374
12	7	0	3.012056	-0.893494	0.000109
13	1	0	3.751827	-0.202411	0.000229
14	1	0	3.271850	-1.870612	0.000574
15	8	0	0.060106	2.632228	0.000069
16	1	0	0.896419	-2.383126	0.000178
17	1	0	0.914047	3.108967	0.000042

Guanine: 1H7H-keto-guanine OHb protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.931772360     A.U.
```

```
 Zero-point correction=                           0.129088
(Hartree/Particle)
 Thermal correction to Energy=                    0.137770
 Thermal correction to Enthalpy=                  0.138714
 Thermal correction to Gibbs Free Energy=         0.095723
 Sum of electronic and zero-point Energies=           -542.802684
 Sum of electronic and thermal Energies=              -542.794003
 Sum of electronic and thermal Enthalpies=            -542.793058
 Sum of electronic and thermal Free Energies=         -542.836049

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.452             34.602             90.482
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.821291	0.439833	-0.000187
2	6	0	0.550692	-0.929757	-0.000017
3	6	0	-1.751580	-0.444966	0.000000
4	6	0	-0.269732	1.338977	0.000003
5	6	0	2.651051	-0.794541	0.000062
6	1	0	3.704572	-1.042358	0.000098
7	7	0	-1.508516	0.866115	0.000038
8	7	0	-0.744136	-1.373917	-0.000119
9	7	0	1.667003	-1.685025	0.000113
10	7	0	2.211169	0.494571	-0.000108
11	1	0	2.810032	1.311332	-0.000107
12	7	0	-3.025751	-0.857454	0.000013
13	1	0	-3.752895	-0.152347	-0.000070
14	1	0	-3.300709	-1.830357	-0.000103
15	8	0	-0.184693	2.665493	0.000050
16	1	0	-0.920660	-2.375417	0.000576
17	1	0	0.728488	2.997893	0.000472

Guanine: 1H7H-keto-guanine N1 protonated
B3LYP/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -542.941575858     A.U.
 Zero-point correction=                           0.129469
(Hartree/Particle)
 Thermal correction to Energy=                    0.138233
 Thermal correction to Enthalpy=                  0.139177
 Thermal correction to Gibbs Free Energy=         0.095976
 Sum of electronic and zero-point Energies=           -542.812107
 Sum of electronic and thermal Energies=              -542.803343
 Sum of electronic and thermal Enthalpies=            -542.802399
 Sum of electronic and thermal Free Energies=         -542.845600

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.743             34.568             90.925
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.865991	0.460786	-0.000324
2	6	0	0.571407	-0.890217	0.000016
3	6	0	-1.758130	-0.459379	0.000131
4	6	0	-0.138284	1.480276	0.000109
5	6	0	2.673968	-0.787970	0.000097
6	1	0	3.722655	-1.052721	0.000176
7	7	0	-1.461075	0.858244	-0.000111
8	7	0	-0.743873	-1.345190	0.000079
9	7	0	1.671296	-1.665279	0.000000
10	7	0	2.244222	0.501026	-0.000092
11	1	0	2.818815	1.337180	-0.000085
12	7	0	-3.030406	-0.876875	-0.000354
13	1	0	-3.803570	-0.223612	0.000612
14	1	0	-3.269326	-1.860772	0.000216
15	8	0	-0.048754	2.685457	0.000080
16	1	0	-0.912126	-2.347031	0.000767
17	1	0	-2.217280	1.538849	0.000849

Guanine: 1H7H-keto-guanine N2 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.883986227 A.U.
Zero-point correction= 0.130071
(Hartree/Particle)
Thermal correction to Energy= 0.138818
Thermal correction to Enthalpy= 0.139762
Thermal correction to Gibbs Free Energy= 0.096233
Sum of electronic and zero-point Energies= -542.753916
Sum of electronic and thermal Energies= -542.745168
Sum of electronic and thermal Enthalpies= -542.744224
Sum of electronic and thermal Free Energies= -542.787753

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.110	33.496	91.614

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.871189	0.444063	0.000307
2	6	0	0.575975	-0.909690	0.000046
3	6	0	-1.651189	-0.318118	-0.000137
4	6	0	-0.125100	1.493133	-0.000039
5	6	0	2.676317	-0.819466	-0.000051
6	1	0	3.724345	-1.086522	-0.000150
7	7	0	-1.465323	0.939551	-0.000005
8	7	0	-0.750992	-1.331389	-0.000084

9	7	0	1.672911	-1.693677	-0.000140
10	7	0	2.248163	0.472599	0.000132
11	1	0	2.822543	1.308806	0.000529
12	7	0	-3.102098	-0.728214	0.000126
13	1	0	-3.627589	0.160855	-0.000422
14	1	0	-3.375671	-1.264770	-0.835842
15	8	0	0.061841	2.689782	-0.000193
16	1	0	-0.964548	-2.324552	-0.000325
17	1	0	-3.375591	-1.263692	0.836809

Guanine: 1H7H-keto-guanine N3H protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.867872097 A.U.
Zero-point correction= 0.128771
(Hartree/Particle)
Thermal correction to Energy= 0.137860
Thermal correction to Enthalpy= 0.138804
Thermal correction to Gibbs Free Energy= 0.094098
Sum of electronic and zero-point Energies= -542.739101
Sum of electronic and thermal Energies= -542.730012
Sum of electronic and thermal Enthalpies= -542.729068
Sum of electronic and thermal Free Energies= -542.773775

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.508	34.297	94.093

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.834803	0.450255	0.000044
2	6	0	-0.585433	-0.894808	0.000099
3	6	0	1.830021	-0.242583	0.000014
4	6	0	0.185266	1.497608	0.000085
5	6	0	-2.675615	-0.764781	-0.000179
6	1	0	-3.729766	-1.005339	-0.000341
7	7	0	1.509384	0.977139	0.000122
8	7	0	0.777089	-1.418987	0.000348
9	7	0	-1.689180	-1.660037	-0.000006
10	7	0	-2.206878	0.513968	-0.000180
11	1	0	-2.755541	1.368910	-0.000240
12	7	0	3.076799	-0.738303	-0.000465
13	1	0	3.844052	-0.073333	-0.000529
14	1	0	3.310420	-1.722510	0.000144
15	8	0	-0.038217	2.684709	0.000080
16	1	0	0.924757	-2.018348	-0.826256
17	1	0	0.924695	-2.017654	0.827471

Guanine: 1H7H-keto-guanine N7H protonated

B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.855322235 A.U.
Zero-point correction= 0.127666
(Hartree/Particle)
Thermal correction to Energy= 0.136831
Thermal correction to Enthalpy= 0.137775
Thermal correction to Gibbs Free Energy= 0.093198
Sum of electronic and zero-point Energies= -542.727656
Sum of electronic and thermal Energies= -542.718492
Sum of electronic and thermal Enthalpies= -542.717548
Sum of electronic and thermal Free Energies= -542.762125

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.862	34.882	93.821

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.741622	0.432287	0.001494
2	6	0	-0.480698	-0.892815	0.000256
3	6	0	1.804514	-0.357388	-0.000038
4	6	0	0.289408	1.468903	-0.000033
5	6	0	-2.633952	-0.898422	-0.000443
6	1	0	-3.691747	-1.135702	-0.000657
7	7	0	1.567414	0.928163	-0.000034
8	7	0	0.794901	-1.345584	-0.000364
9	7	0	-1.644483	-1.692185	-0.000675
10	7	0	-2.200869	0.558165	0.000646
11	1	0	-2.555045	1.070812	-0.825325
12	7	0	3.070673	-0.811644	0.000975
13	1	0	3.813502	-0.123384	-0.000788
14	1	0	3.323338	-1.789694	-0.003076
15	8	0	0.016829	2.659419	-0.000964
16	1	0	0.992333	-2.341110	-0.000291
17	1	0	-2.556363	1.069925	0.826582

Guanine: 1H7H-keto-guanine N9 protonated
B3LYP/6-31+G*

SCF Done: E(RB+HF-LYP) = -542.914895025 A.U.
Zero-point correction= 0.128947
(Hartree/Particle)
Thermal correction to Energy= 0.137824
Thermal correction to Enthalpy= 0.138769
Thermal correction to Gibbs Free Energy= 0.095228
Sum of electronic and zero-point Energies= -542.785949
Sum of electronic and thermal Energies= -542.777071
Sum of electronic and thermal Enthalpies= -542.776127
Sum of electronic and thermal Free Energies= -542.819667

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.486	34.745	91.638

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.763998	0.462424	0.004901
2	6	0	-0.499717	-0.880173	-0.005552
3	6	0	1.793116	-0.366858	0.009290
4	6	0	0.305735	1.475448	-0.002708
5	6	0	-2.703944	-0.614555	0.002803
6	1	0	-3.761559	-0.833449	-0.000103
7	7	0	1.575605	0.917014	0.021142
8	7	0	0.779619	-1.355619	0.013979
9	7	0	-1.712597	-1.540175	-0.002739
10	7	0	-2.138877	0.588668	0.010009
11	1	0	-2.626219	1.482916	0.014637
12	7	0	3.056322	-0.844972	-0.038983
13	1	0	3.795163	-0.153428	0.017412
14	1	0	3.292406	-1.788870	0.236855
15	8	0	0.058437	2.668008	-0.017268
16	1	0	0.997875	-2.320704	-0.205326
17	1	0	-1.872818	-2.542666	-0.001598

CPCM CALCULATIONS

1,N^6-ethenoadenine: NEUTRAL N9H

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -543.559834951 A.U.

Total free energy in solution: with all non electrostatic terms	(a.u.) =	-543.558208
(Polarized solute)-Solvent	(kcal/mol) =	-25.93
Cavitation energy	(kcal/mol) =	18.60
Dispersion energy	(kcal/mol) =	-22.38
Repulsion energy	(kcal/mol) =	4.80
Total non electrostatic	(kcal/mol) =	1.02

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.851121	-0.943500	0.000011
2	6	0	-2.709810	0.420105	0.000103
3	6	0	-0.723972	-0.625728	-0.000011
4	6	0	-0.633632	1.832392	0.000033
5	6	0	1.292301	0.678674	-0.000061

6	6	0	2.802728	-0.918304	0.000009
7	7	0	0.670834	1.886689	0.000003
8	7	0	-1.336193	0.647546	0.000029
9	7	0	-1.629177	-1.591524	-0.000072
10	7	0	2.645310	0.436783	0.000170
11	7	0	1.652234	-1.576894	-0.000280
12	6	0	0.694406	-0.586726	-0.000044
13	1	0	3.784514	-1.378715	0.000064
14	1	0	3.397769	1.143809	0.000404
15	1	0	-1.226598	2.744419	0.000120
16	1	0	-3.422793	1.235370	0.000198
17	1	0	-3.779339	-1.504561	0.000020

1,N^6-ethenoadenine: N9H N9 deprotonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -543.090887086 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-543.089462
(Polarized solute)-Solvent	(kcal/mol) =	-71.63
Cavitation energy	(kcal/mol) =	18.31
Dispersion energy	(kcal/mol) =	-21.96
Repulsion energy	(kcal/mol) =	4.55
Total non electrostatic	(kcal/mol) =	0.89

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.813939	-0.953359	0.000085
2	6	0	-2.676530	0.410946	0.000078
3	6	0	-0.681481	-0.622673	-0.000030
4	6	0	-0.601028	1.832162	0.000150
5	6	0	1.360603	0.687732	-0.000016
6	6	0	2.839213	-0.833888	-0.000234
7	7	0	0.702121	1.890526	0.000058
8	7	0	-1.301492	0.641914	0.000052
9	7	0	-1.590412	-1.597609	0.000034
10	7	0	2.717580	0.512691	-0.000076
11	7	0	1.694633	-1.557336	-0.000082
12	6	0	0.734285	-0.580957	-0.000022
13	1	0	3.812902	-1.317071	-0.000095
14	1	0	-1.202898	2.738668	0.000073
15	1	0	-3.392269	1.224090	-0.000032
16	1	0	-3.741485	-1.516762	0.000083

1,N^6-ethenoadenine: N9H N10 protonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

```
SCF Done:  E(RB+HF-LYP) =  -544.009999235     A.U.
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -544.008169
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -66.00
 ---------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      18.84
 Dispersion energy                         (kcal/mol) =     -22.80
 Repulsion energy                          (kcal/mol) =       5.11
 Total non electrostatic                   (kcal/mol) =       1.15
 ---------------------------------------------------------------------

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.894543   -0.851177   -0.000149
    2          6             0       -2.687170    0.490249   -0.000421
    3          6             0       -0.686400   -0.561062   -0.000041
    4          6             0       -0.579405    1.862271    0.000147
    5          6             0        1.332436    0.685683    0.000272
    6          6             0        2.807252   -0.941164   -0.000462
    7          7             0        0.722926    1.893247    0.000632
    8          7             0       -1.299122    0.680420   -0.000281
    9          7             0       -1.661490   -1.482878    0.000568
   10          7             0        2.673007    0.419181    0.000343
   11          7             0        1.649994   -1.584079   -0.000708
   12          6             0        0.715751   -0.577817   -0.000177
   13          1             0        3.440277    1.115050    0.000842
   14          1             0        3.782663   -1.416037   -0.000686
   15          1             0       -1.168004    2.777347    0.000394
   16          1             0       -3.817431   -1.416127    0.000137
   17          1             0       -3.374839    1.325421   -0.000763
   18          1             0       -1.507398   -2.508787    0.001184
 ---------------------------------------------------------------------
```

Cytosine: NEUTRAL C1

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

```
SCF Done:  E(RB+HF-LYP) =  -394.988472192     A.U.
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -394.987208
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -32.66
 ---------------------------------------------------------------------
```

```
 Cavitation energy                        (kcal/mol) =      14.40
 Dispersion energy                        (kcal/mol) =     -18.02
 Repulsion energy                         (kcal/mol) =       4.41
 Total non electrostatic                  (kcal/mol) =       0.79
 -------------------------------------------------------------------

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.201165    1.708567    0.000028
    2          6             0        1.052922    1.180735   -0.000641
    3          6             0        1.145946   -0.253389   -0.000187
    4          6             0       -1.180587   -0.505651    0.000024
    5          7             0       -1.288193    0.890921    0.000442
    6          1             0       -0.402200    2.776567    0.000129
    7          1             0        1.937847    1.810246   -0.001141
    8          7             0        2.356614   -0.841917   -0.000422
    9          8             0       -2.224583   -1.187728   -0.000158
   10          1             0       -2.238882    1.288856    0.001868
   11          1             0        3.215421   -0.293740    0.004661
   12          1             0        2.429503   -1.858998    0.002162
   13          7             0        0.067618   -1.049386   -0.000271
 -------------------------------------------------------------------
```

Cytosine: N1 deprotonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

```
SCF Done:  E(RB+HF-LYP) =  -394.511725950     A.U.
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -394.510768
 -------------------------------------------------------------------
 (Polarized solute)-Solvent               (kcal/mol) =     -90.67
 -------------------------------------------------------------------
 Cavitation energy                        (kcal/mol) =      13.94
 Dispersion energy                        (kcal/mol) =     -18.20
 Repulsion energy                         (kcal/mol) =       4.87
 Total non electrostatic                  (kcal/mol) =       0.60
 -------------------------------------------------------------------

-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.245846    1.697277    0.003454
    2          6             0        1.036290    1.171068   -0.000775
    3          6             0        1.116695   -0.241857   -0.005975
    4          6             0       -1.219514   -0.409909    0.000024
    5          7             0       -1.369883    0.963640    0.002638
    6          1             0       -0.385317    2.781460    0.009614
    7          1             0        1.923152    1.800067   -0.001191
    8          7             0        2.334255   -0.879189   -0.064158
```

9	8	0	-2.257772	-1.145244	0.003961
10	1	0	3.159277	-0.349866	0.228202
11	1	0	2.342932	-1.866454	0.205216
12	7	0	0.020826	-1.013413	-0.003322

Cytosine: N3 protonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -395.442386072 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-395.441305
(Polarized solute)-Solvent	(kcal/mol) =	-81.26
Cavitation energy	(kcal/mol) =	14.52
Dispersion energy	(kcal/mol) =	-18.79
Repulsion energy	(kcal/mol) =	4.95
Total non electrostatic	(kcal/mol) =	0.68

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.208172	1.724274	-0.000068
2	6	0	1.054012	1.211268	-0.000388
3	6	0	1.196522	-0.206338	-0.000485
4	6	0	-1.239737	-0.459983	0.000075
5	7	0	-1.306617	0.920683	0.000321
6	1	0	-0.406148	2.793043	-0.000149
7	1	0	1.929584	1.851034	-0.000517
8	7	0	2.370647	-0.815122	-0.000043
9	8	0	-2.221662	-1.188854	0.000820
10	1	0	-2.257644	1.334387	0.000760
11	1	0	3.239074	-0.271774	0.002447
12	1	0	2.448172	-1.838060	-0.000552
13	7	0	0.060199	-0.959198	-0.000712
14	1	0	0.134910	-1.997661	-0.000322

Cytosine: O protonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -395.426411237 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-395.425520

```
 (Polarized solute)-Solvent               (kcal/mol) =     -68.53
 ---------------------------------------------------------------------
 Cavitation energy                        (kcal/mol) =      14.56
 Dispersion energy                        (kcal/mol) =     -18.97
 Repulsion energy                         (kcal/mol) =       4.96
 Total non electrostatic                  (kcal/mol) =       0.56
 ---------------------------------------------------------------------

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.082041    1.744058   -0.000159
    2          6             0        1.142457    1.153024   -0.001734
    3          6             0        1.182775   -0.279832   -0.000277
    4          6             0       -1.106024   -0.375900    0.000303
    5          7             0       -1.212972    0.975087    0.001970
    6          1             0       -0.237319    2.818814   -0.000691
    7          1             0        2.054784    1.743864   -0.003779
    8          7             0        2.335644   -0.942120    0.000656
    9          8             0       -2.262488   -1.016935   -0.001186
   10          1             0       -2.154016    1.414591    0.004113
   11          1             0        3.232336   -0.451267    0.002562
   12          1             0        2.341711   -1.964908    0.002405
   13          7             0        0.039888   -1.014847   -0.000131
   14          1             0       -2.098509   -2.000565   -0.001386
 ---------------------------------------------------------------------
```

Adenine: NEUTRAL N9H amino

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

```
SCF Done:  E(RB+HF-LYP) =  -467.369454805     A.U.
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -467.368315
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent               (kcal/mol) =     -22.53
 ---------------------------------------------------------------------
 Cavitation energy                        (kcal/mol) =      16.44
 Dispersion energy                        (kcal/mol) =     -20.57
 Repulsion energy                         (kcal/mol) =       4.85
 Total non electrostatic                  (kcal/mol) =       0.72
 ---------------------------------------------------------------------

-----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.723005    0.764557    0.000425
    2          6             0       -0.174722   -0.524386   -0.002087
    3          6             0        1.237165   -0.610396   -0.001888
    4          6             0        1.284162    1.712997    0.000914
    5          6             0       -2.292701   -0.783358    0.000372
```

6	1	0	1.910978	2.604002	0.002590
7	1	0	-3.294036	-1.200483	0.001049
8	7	0	1.946458	0.542727	0.000276
9	7	0	-0.036174	1.922602	0.001487
10	7	0	-1.175452	-1.484554	-0.001932
11	7	0	-2.082604	0.572591	0.002026
12	7	0	1.902774	-1.784204	-0.028787
13	1	0	2.915332	-1.785456	0.090818
14	1	0	1.406648	-2.663737	0.104736
15	1	0	-2.809350	1.305062	0.002906

Adenine: N9H N9 deprotonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -466.899462758 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-466.898524
(Polarized solute)-Solvent	(kcal/mol) =	-71.73
Cavitation energy	(kcal/mol) =	16.07
Dispersion energy	(kcal/mol) =	-20.36
Repulsion energy	(kcal/mol) =	4.89
Total non electrostatic	(kcal/mol) =	0.59

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276029	1.696877	0.002297
2	7	0	0.035728	1.926110	0.002162
3	6	0	0.778407	0.784910	0.001033
4	6	0	0.218598	-0.515357	-0.005140
5	6	0	-1.184780	-0.623357	-0.004844
6	7	0	-1.922780	0.510587	0.000644
7	7	0	1.236889	-1.447888	-0.005312
8	7	0	-1.841876	-1.823529	-0.060909
9	6	0	2.331665	-0.665103	0.001732
10	1	0	-1.326790	-2.659527	0.221811
11	1	0	-2.830663	-1.816803	0.200840
12	1	0	3.332670	-1.090515	0.004526
13	1	0	-1.922236	2.575198	0.005334
14	7	0	2.140589	0.680981	0.005847

Adenine: N9H N1 protonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -467.821109332 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-467.820385
(Polarized solute)-Solvent	(kcal/mol) =	-77.38
Cavitation energy	(kcal/mol) =	16.45
Dispersion energy	(kcal/mol) =	-21.56
Repulsion energy	(kcal/mol) =	5.56
Total non electrostatic	(kcal/mol) =	0.45

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745411	0.763365	0.000512
2	6	0	-0.220643	-0.536030	0.000035
3	6	0	1.183610	-0.679389	-0.000369
4	6	0	1.248502	1.739403	0.000171
5	6	0	-2.333606	-0.755214	-0.000426
6	1	0	1.926776	2.589720	0.000339
7	1	0	-3.341977	-1.155227	-0.000890
8	7	0	1.859859	0.513049	-0.000658
9	7	0	-0.044944	1.923803	0.000799
10	7	0	-1.228099	-1.475294	0.000006
11	7	0	-2.098111	0.596764	0.000240
12	7	0	1.843894	-1.828515	-0.000372
13	1	0	2.867919	-1.861508	-0.000630
14	1	0	1.334868	-2.715892	0.002275
15	1	0	-2.812005	1.346890	0.000072
16	1	0	2.901515	0.494551	-0.000814

Adenine: N9H N3 protonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -467.817655377 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-467.816891
(Polarized solute)-Solvent	(kcal/mol) =	-77.37
Cavitation energy	(kcal/mol) =	16.46
Dispersion energy	(kcal/mol) =	-21.61
Repulsion energy	(kcal/mol) =	5.63
Total non electrostatic	(kcal/mol) =	0.48

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742958	0.722871	0.000510
2	6	0	-0.188638	-0.555078	-0.000014
3	6	0	1.225915	-0.664217	-0.000189
4	6	0	1.372819	1.654098	-0.000412
5	6	0	-2.307426	-0.798861	-0.000543
6	1	0	1.973938	2.561313	-0.000653
7	1	0	-3.314228	-1.202528	-0.001026
8	7	0	1.970001	0.486240	-0.000871
9	7	0	0.029739	1.840108	0.000680
10	7	0	-1.195799	-1.501906	-0.000379
11	7	0	-2.087759	0.563342	0.000302
12	7	0	1.870678	-1.825112	0.000264
13	1	0	2.893326	-1.843527	0.000902
14	1	0	1.367025	-2.714207	0.003646
15	1	0	-2.809699	1.308096	0.000055
16	1	0	-0.376651	2.799277	0.001003

Guanine: NEUTRAL 9H-keto

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

```
SCF Done:  E(RB+HF-LYP) =  -542.625358415     A.U.
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -542.624023
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -40.94
 ---------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      17.66
 Dispersion energy                         (kcal/mol) =     -22.46
 Repulsion energy                          (kcal/mol) =       5.64
 Total non electrostatic                   (kcal/mol) =       0.84
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.841862	0.504773	-0.000752
2	6	0	-0.537418	-0.860317	0.000344
3	6	0	1.678823	-0.573213	-0.000643
4	6	0	0.234019	1.445836	0.000483
5	6	0	-2.718047	-0.516318	0.001061
6	1	0	-3.773852	-0.763469	0.001428
7	7	0	1.482877	0.789255	0.000463
8	1	0	2.308896	1.412008	-0.009173
9	7	0	0.682645	-1.446393	0.003499
10	7	0	-2.215207	0.699548	-0.000286
11	7	0	-1.749926	-1.495313	0.001695

12	1	0	-1.907920	-2.514728	0.001820
13	8	0	0.187464	2.686293	0.001625
14	7	0	2.963297	-1.011155	-0.058451
15	1	0	3.719569	-0.381196	0.213637
16	1	0	3.114709	-1.999129	0.147890

Guanine: 9H-keto N9 deprotonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -542.155888903 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-542.154593
(Polarized solute)-Solvent	(kcal/mol) =	-92.24
Cavitation energy	(kcal/mol) =	17.31
Dispersion energy	(kcal/mol) =	-22.29
Repulsion energy	(kcal/mol) =	5.79
Total non electrostatic	(kcal/mol) =	0.81

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.881912	0.461746	-0.000366
2	6	0	0.572607	-0.916390	-0.001025
3	6	0	-1.658598	-0.553983	-0.002396
4	6	0	-0.164492	1.423002	0.000296
5	6	0	2.684008	-0.655155	0.003444
6	7	0	-1.431667	0.804709	-0.002829
7	1	0	-2.245541	1.448971	-0.017834
8	7	0	-0.694805	-1.448653	0.002942
9	7	0	2.257487	0.614806	0.002192
10	7	0	1.729209	-1.631185	0.000633
11	8	0	-0.096710	2.673451	0.001747
12	7	0	-2.975717	-0.948209	-0.074947
13	1	0	-3.672433	-0.304654	0.312493
14	1	0	-3.135026	-1.923549	0.191136
15	1	0	3.742511	-0.903973	0.004566

Guanine: 9H-keto N7 protonated

B3LYP/6-31+G* OPT(maxcyc=10) SCRF(read, CPCM, solvent=water) RADII=UAKS

SCF Done: E(RB+HF-LYP) = -543.074389496 A.U.
Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-543.073443

(Polarized solute)-Solvent (kcal/mol) =	-84.86
Cavitation energy (kcal/mol) =	17.63
Dispersion energy (kcal/mol) =	-23.37
Repulsion energy (kcal/mol) =	6.33
Total non electrostatic (kcal/mol) =	0.59

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.786976	0.482248	-0.000785
2	6	0	0.487505	-0.874721	-0.000265
3	6	0	-1.722317	-0.558031	-0.000340
4	6	0	-0.266320	1.451450	0.000013
5	6	0	2.695048	-0.621316	0.000346
6	1	0	3.755203	-0.849430	0.000547
7	7	0	-1.513556	0.806347	-0.000564
8	1	0	-2.336878	1.437677	0.000791
9	7	0	-0.725913	-1.444552	0.000009
10	7	0	2.166769	0.597344	-0.000712
11	7	0	1.704481	-1.531913	0.000279
12	1	0	1.842335	-2.561773	0.000261
13	8	0	-0.172328	2.681559	0.001790
14	7	0	-2.992068	-0.985531	-0.000170
15	1	0	-3.783096	-0.339919	-0.001367
16	1	0	-3.177779	-1.988947	0.000984
17	1	0	2.715496	1.480276	-0.001249