Theoretical Bond Dissociation Energies of Halo-Heterocycles: Trends and Relationships to Regioselectivity in Palladium-Catalyzed Cross-Coupling Reactions.

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Full reference 11

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.;Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, 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. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; 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. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Pittsburgh PA, 2003

Table of Content

Table S1. Summary of BDEs of various mono-chloro heterocycles. Energies in kcal/mol.

	BDE G3B3	BDE B3LYP
2-chlorofuran	102.0	95.5
3-chlorofuran	101.4	95.5
2-chloropyrrole	101.9	96.3
3-chloropyrrole	101.5	96.3
2-chlorothiophene	98.8	92.5
3-chlorothiophene	98.6	92.2
2-chloroimidazole	99.4	93.3
4-chloroimidazole	100.4	94.3
5-chloroimidazole	101.3	95.4
2-chlorooxazole	100.3	94.0
4-chlorooxazole	101.1	94.3
5-chlorooxazole	102.3	95.7
2-chlorothiazole	93.7	87.4
4-chlorothiazole	97.8	90.8
5-chlorothiazole	98.8	92.4
3-chloroisothiazole	94.7	87.9
4-chloroisothiazole	98.6	92.1
5-chloroisothiazole	97.9	91.5
3-chloropyrazole	100.3	94.3
4-chloropyrazole	101.5	95.9
5-chloropyrazole	101.1	95.0
3-chloroisoxazole	99.0	92.2
4-chloroisoxazole	103.6	95.2
5-chloroisoxazole	100.5	93.4
4-chloro-1,2,3-triazole	102.1	94.7
5-chloro-1,2,3-triazole	101.9	94.8
3-chloro1,2,4-triazole	100.7	94.5
5-chloro1,2,4-triazole	99.9	93.5
3-chloro-1,2,4-oxadiazole	99.9	93.1
5-chloro-1,2,4-oxadiazole	99.8	93.3
3-chloro-1,2,5-oxadiazole	100.9	93.2
2-chloro-1,3,4-oxadiazole	101.3	94.5
4-chloro-1,2,3,5-oxatriazole	103.9	95.3
2-chloropyridine	94.9	87.1
3-chloropyridine	99.2	90.6
4-chloropyridine	98.4	89.9

4-chloropyridazine	93.3	86.7
4-chloropyridazine	94.7	87.9
2-chloropyrimidine	95.1	87.6
4-chloropyrimidine	93.7	86.0
5-chloropyrimidine	99.0	90.6
2-chloropyrazine	92.9	86.3
2-chloro-1,3,5-triazine	92.7	86.6
3-chloro-1,3,5-triazine	93.7	87.3
5-chloro-1,3,5-triazine	90.6	83.8
6-chloro-1,3,5-triazine	93.0	86.1
4-chloro-1,2,3-triazine	91.6	84.6
5-chloro-1,2,3-triazine	93.8	86.8

Table S2. Spin distribution of radicals

Computational Details

All the molecular calculations were performed with the Gaussian 03 suite of programs. Geometry optimizations of the model systems in the gas phase were carried out with the B3LYP/6-31G(d) DFT method[1] or the G3B3 method.[2] Frequency calculations were performed to verify the nature of all the stationary points as either minima or transition states and to provide zero point energy corrections.

Error Analysis

Bootstrapping with 10.000 samples was applied to determine the mean for slope, intercept and correlation coefficient (R^2) using MATLAB[3]. The standard deviations were then calculated.

[1] 1 (a) Kohn, W.; Becke, A. D.; Parr, R. G., *J. Phys. Chem.* **1996**, *100*, 12974. (b) Becke, A. D., *J. Chem. Phys.* **1993**, *98*, 5648.
[2] Baboul, A. G.; Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Journal of Chemical Physics 1999, 110, 7650.
[3] (© 1994-2009 The MathWorks, Inc.)

Molecular Geometries: *B3LYP/6-31g(d)*

Chlorofurans

Supporting Information: **23dichlorofuran.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C4H2Cl2O   C1[X(C4H2Cl2O)]  #Atoms= 9
 Charge = 0     Multiplicity = 1
---------------------------------------------------------------------
 SCF Energy= -1149.20160382     Predicted Change= -6.159808D-07
=====================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00042 ||  0.00045   [ YES ]      0.00010 ||  0.00030   [ YES ]
 Displ      0.00162 ||  0.00180   [ YES ]      0.00162 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic        Coordinates (Angstroms)
      Type      X          Y      Z
---------------------------------------------------------------------
      C        0.649092      0.028451     -0.000073
      C       -0.697381      0.249300      0.000013
      C       -0.874667      1.671954     -0.000303
      C        0.376976      2.199091      0.000290
      H       -1.815018      2.203327     -0.000463
      H        0.764706      3.205585      0.000568
      O        1.320657      1.207643     -0.000078
      Cl       1.577100     -1.406111     -0.000008
      Cl      -1.944104     -0.944644      0.000065
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -1149.20160382 Predicted Change= -6.159808D-07
 Zero-point correction (ZPE)=        -1149.1501  0.05145
 Internal Energy (U)=               -1149.1442  0.05736
 Enthalpy (H)=                     -1149.1432   0.05830
 Gibbs Free Energy (G)=             -1149.1811    0.02040
---------------------------------------------------------------------
 Frequencies --   166.9349              200.4057              254.4006
```

Supporting Information: **24dichlorofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Cl2O C1[X(C4H2Cl2O)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1149.20261074 Predicted Change= -6.107650D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00059	0.00180	[YES]	0.00059	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.631204	1.319496	0.000174
C	1.125573	0.052123	-0.000157
C	0.012355	-0.850998	0.000257
C	-1.080943	-0.040951	0.000150
H	1.078239	2.300039	0.000218
H	0.034860	-1.929805	0.000357
O	-0.737616	1.270488	0.000205
Cl	2.798390	-0.396672	-0.000524
Cl	-2.759644	-0.392278	0.000244

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1149.20261074 Predicted Change= -6.107650D-08
Zero-point correction (ZPE)= -1149.1512 0.05132
Internal Energy (U)= -1149.1453 0.05725
Enthalpy (H)= -1149.1444 0.05819
Gibbs Free Energy (G)= -1149.1823 0.02027

Frequencies -- 145.9445 201.4910 308.4873

Supporting Information: **2chloro3radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -688.911255026 Predicted Change= -5.092640D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00045	0.00180	[YES]	0.00045	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.647829	0.017251	-0.000076
C	-0.680628	0.263910	-0.000318
C	-0.887040	1.672408	-0.000148
C	0.372870	2.194904	0.000131
H	-1.820392	2.215993	-0.000267
H	0.760036	3.202475	0.000323
O	1.323995	1.206971	0.000329
Cl	1.584795	-1.414672	-0.000027

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -688.911255026 Predicted Change= -5.092640D-08
Zero-point correction (ZPE)= -688.8630 0.04815
Internal Energy (U)= -688.8583 0.05290
Enthalpy (H)= -688.8574 0.05384
Gibbs Free Energy (G)= -688.8924 0.01882

Frequencies -- 208.7715 313.7409 494.8119

Supporting Information: **2chloro4radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -688.913243602 Predicted Change= -3.113175D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00089	0.00180	[YES]	0.00089	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.240734	0.107022	0.000108
C	0.591616	1.189777	-0.000309
C	1.885014	0.596415	0.000297
C	1.781980	-0.749168	0.000039
H	0.311054	2.231634	-0.000470
H	2.464806	-1.582029	0.000132
O	0.434373	-1.069635	-0.000404
Cl	-1.954548	-0.008185	0.000159

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -688.913243602 Predicted Change= -3.113175D-07
Zero-point correction (ZPE)= -688.8651 0.04808
Internal Energy (U)= -688.8604 0.05282
Enthalpy (H)= -688.8594 0.05377
Gibbs Free Energy (G)= -688.8944 0.01876

Frequencies -- 223.2993 315.6892 489.2900

Supporting Information: **2chlorofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClO C1[X(C4H3ClO)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -689.612052325 Predicted Change= -8.280486D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.245110	0.103410	0.000031
C	0.595975	1.173034	-0.000260
C	1.918080	0.613205	0.000225
C	1.766282	-0.737739	0.000015
H	0.312791	2.215033	-0.000420
H	2.852926	1.156138	0.000467
H	2.449007	-1.572893	0.000069
O	0.436357	-1.068887	-0.000182
Cl	-1.959821	-0.009332	0.000075

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -689.612052325 Predicted Change= -8.280486D-08
Zero-point correction (ZPE)= -689.5512 0.06078
Internal Energy (U)= -689.5465 0.06554
Enthalpy (H)= -689.5455 0.06648
Gibbs Free Energy (G)= -689.5799 0.03207

Frequencies -- 222.7153 313.0202 490.6118

Supporting Information: **3chlorofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClO C1[X(C4H3ClO)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -689.612143265 Predicted Change= -7.852386D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00089	0.00180	[YES]	0.00089	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.525967	-1.098042	0.000265
C	0.274453	0.003474	-0.000045
C	-0.580378	1.153317	0.000344
C	-1.846141	0.655583	-0.000257
H	-0.332786	-2.158720	0.000400
H	-0.277794	2.190144	0.000586
H	-2.823499	1.113136	-0.000495
O	-1.831522	-0.707909	-0.000093
Cl	2.009086	0.013690	-0.000094

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -689.612143265 Predicted Change= -7.852386D-08
Zero-point correction (ZPE)= -689.5512 0.06091
Internal Energy (U)= -689.5464 0.06567
Enthalpy (H)= -689.5455 0.06662
Gibbs Free Energy (G)= -689.5799 0.03217

Frequencies -- 249.9773 294.0200 476.6345

Supporting Information: **3chlorofuranradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3O(2) C1[X(C4H3O)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -229.321688517 Predicted Change= -4.417062D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00143	0.00180	[YES]	0.00143	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.514845	-1.106956	0.000256
C	0.255277	0.003595	-0.000328
C	-0.572597	1.161807	0.000526
C	-1.840368	0.655687	-0.000467
H	-0.335884	-2.169464	0.000229
H	-0.283252	2.202443	0.000764
H	-2.818549	1.113316	-0.000836
O	-1.833417	-0.709444	0.000562

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -229.321688517 Predicted Change= -4.417062D-07
Zero-point correction (ZPE)= -229.2641 0.05751
Internal Energy (U)= -229.2604 0.06121
Enthalpy (H)= -229.2595 0.06216
Gibbs Free Energy (G)= -229.2910 0.03067

Frequencies -- 546.0974 616.8987 695.5559

Supporting Information: **4chloro2radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -688.912883659 Predicted Change= -2.548945D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00106	0.00180	[YES]	0.00106	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.520768	-1.105494	-0.000205
C	0.270673	0.001852	0.000422
C	-0.577897	1.169674	-0.000092
C	-1.822996	0.631476	0.000448
H	-0.338549	-2.167588	-0.000492
H	-0.281227	2.206189	-0.000269
O	-1.843330	-0.699884	0.000648
Cl	2.003046	0.015313	0.000648

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -688.912883659 Predicted Change= -2.548945D-07
Zero-point correction (ZPE)= -688.8650 0.04787
Internal Energy (U)= -688.8602 0.05266
Enthalpy (H)= -688.8592 0.05360
Gibbs Free Energy (G)= -688.8943 0.01851

Frequencies -- 247.9059 296.9995 475.6145

Supporting Information: **2chloro3radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -688.911255026 Predicted Change= -5.092640D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00045	0.00180	[YES]	0.00045	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.647829	0.017251	-0.000076
C	-0.680628	0.263910	-0.000318
C	-0.887040	1.672408	-0.000148
C	0.372870	2.194904	0.000131
H	-1.820392	2.215993	-0.000267
H	0.760036	3.202475	0.000323
O	1.323995	1.206971	0.000329
Cl	1.584795	-1.414672	-0.000027

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -688.911255026 Predicted Change= -5.092640D-08
Zero-point correction (ZPE)= -688.8630 0.04815
Internal Energy (U)= -688.8583 0.05290
Enthalpy (H)= -688.8574 0.05384
Gibbs Free Energy (G)= -688.8924 0.01882

Frequencies -- 208.7715 313.7409 494.8119

Supporting Information: **2chloro4radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -688.913243602 Predicted Change= -3.113175D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00089	0.00180	[YES]	0.00089	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.240734	0.107022	0.000108
C	0.591616	1.189777	-0.000309
C	1.885014	0.596415	0.000297
C	1.781980	-0.749168	0.000039
H	0.311054	2.231634	-0.000470
H	2.464806	-1.582029	0.000132
O	0.434373	-1.069635	-0.000404
Cl	-1.954548	-0.008185	0.000159

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -688.913243602 Predicted Change= -3.113175D-07
Zero-point correction (ZPE)= -688.8651 0.04808
Internal Energy (U)= -688.8604 0.05282
Enthalpy (H)= -688.8594 0.05377
Gibbs Free Energy (G)= -688.8944 0.01876

Frequencies -- 223.2993 315.6892 489.2900

Supporting Information: **furan.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4O C1[X(C4H4O)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -230.020581591 Predicted Change= -1.545275D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.094704	-0.348288	-0.000025
C	-0.718703	0.959236	0.000119
C	0.717150	0.960338	-0.000174
C	1.095249	-0.346585	0.000174
H	-2.049428	-0.851751	0.000008
H	1.372101	1.820505	-0.000260
H	2.050780	-0.848514	0.000309
O	0.000961	-1.160843	-0.000105
H	-1.375089	1.818301	0.000218

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -230.020581591 Predicted Change= -1.545275D-07
Zero-point correction (ZPE)= -229.9503 0.07020
Internal Energy (U)= -229.9466 0.07391
Enthalpy (H)= -229.9457 0.07486
Gibbs Free Energy (G)= -229.9766 0.04393

Frequencies -- 613.8315 622.8532 722.6649

Chlorooxatriazoles

Supporting Information: **4chloro1235oxatriazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= CClN3O C1[X(CClN3O)] #Atoms= 6

Charge = 0 Multiplicity = 1

SCF Energy= -737.661553111 Predicted Change= -8.972320D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00042	0.00045	[YES]	0.00014	0.00030	[YES]
Displ	0.00100	0.00180	[YES]	0.00100	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.217092	-0.026018	-0.000404
O	1.774732	-0.658651	-0.000218
N	1.760174	0.747653	-0.000026
N	0.558459	1.117736	0.000396
N	0.498633	-1.117421	0.000448
Cl	-1.918598	0.011149	-0.000092

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.661553111 Predicted Change= -8.972320D-07

Zero-point correction (ZPE)= -737.6376 0.02386

Internal Energy (U)= -737.6333 0.02824

Enthalpy (H)= -737.6323 0.02919

Gibbs Free Energy (G)= -737.6661 -0.00461

Frequencies -- 268.8014 327.1403 512.3390

Supporting Information: **4radical1235oxatriazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= CN3O(2) C1[X(CN3O)] #Atoms= 5
Charge = 0 Multiplicity = 2

SCF Energy= -277.371134003 Predicted Change= -5.339342D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00015	0.00030	[YES]
Displ	0.00087	0.00180	[YES]	0.00087	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.162179	1.112467	0.000112
O	0.540548	-0.924534	-0.000092
N	-0.853189	-0.724599	0.000224
N	-1.069737	0.521896	-0.000243
N	1.166146	0.305772	0.000029

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -277.371134003 Predicted Change= -5.339342D-07
Zero-point correction (ZPE)= -277.3510 0.02010
Internal Energy (U)= -277.3476 0.02351
Enthalpy (H)= -277.3466 0.02445
Gibbs Free Energy (G)= -277.3776 -0.00655

Frequencies -- 619.1436 639.8160 684.9325

Chlorotriazines

Supporting Information: **4chloro123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -739.890951584 Predicted Change= -4.308697D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00115	0.00180	[YES]	0.00115	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.148023	-1.174295	0.000025
C	0.455038	0.009832	0.000010
C	-0.240940	1.213303	-0.000012
C	-1.618484	1.066970	-0.000019
N	-2.217376	-0.135330	0.000038
H	0.253494	2.177863	-0.000004
H	-2.287159	1.923753	0.000018
N	-1.479651	-1.230846	-0.000010
Cl	2.198549	-0.003468	-0.000015

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -739.890951584 Predicted Change= -4.308697D-07

Zero-point correction (ZPE)= -739.8371 0.05381

Internal Energy (U)= -739.8318 0.05910

Enthalpy (H)= -739.8309 0.06004

Gibbs Free Energy (G)= -739.8669 0.02404

Frequencies -- 161.0712 308.7783 346.7186

Supporting Information: **4radical123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -279.617474175 Predicted Change= -2.088777D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00094	0.00180	[YES]	0.00094	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.131767	-1.152680	0.000011
C	0.434068	-0.002454	0.000002
C	-0.231922	1.218441	-0.000003
C	-1.610204	1.068519	0.000004
N	-2.203222	-0.144664	0.000016
H	0.256775	2.186874	-0.000005
H	-2.288795	1.918440	0.000006
N	-1.508034	-1.241226	0.000015

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -279.617474175 Predicted Change= -2.088777D-07
Zero-point correction (ZPE)= -279.5674 0.05003
Internal Energy (U)= -279.5631 0.05432
Enthalpy (H)= -279.5622 0.05526
Gibbs Free Energy (G)= -279.5954 0.02200

Frequencies -- 294.0923 400.2499 573.4575

Supporting Information: **5chloro123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -739.889064357 Predicted Change= -2.707878D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.593987	-1.154438	0.000006
C	-0.255087	-1.176003	-0.000001
C	0.482987	-0.000001	-0.000004
C	-0.255089	1.176004	-0.000003
N	-1.593985	1.154441	0.000010
H	0.213170	-2.156507	-0.000006
H	0.213172	2.156506	0.000001
N	-2.245496	-0.000002	0.000004
Cl	2.221827	0.000000	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -739.889064357 Predicted Change= -2.707878D-07
Zero-point correction (ZPE)= -739.8351 0.05393
Internal Energy (U)= -739.8298 0.05925
Enthalpy (H)= -739.8288 0.06019
Gibbs Free Energy (G)= -739.8649 0.02412

Frequencies -- 164.0609 285.5443 381.5774

Supporting Information: **5radical123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -279.612342445 Predicted Change= -3.181391D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00040 ‖	0.00180	[YES]	0.00040 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.598741	-1.150241	0.000004
C	-0.239500	-1.179841	-0.000001
C	0.458637	0.000000	-0.000004
C	-0.239500	1.179841	-0.000003
N	-1.598740	1.150242	0.000006
H	0.202816	-2.171480	-0.000005
H	0.202817	2.171479	0.000003
N	-2.222105	0.000000	0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -279.612342445 Predicted Change= -3.181391D-08
Zero-point correction (ZPE)= -279.5618 0.05051
Internal Energy (U)= -279.5576 0.05469
Enthalpy (H)= -279.5567 0.05563
Gibbs Free Energy (G)= -279.5897 0.02257

Frequencies -- 362.5321 365.9292 581.7408

Chlorotriazoles

Supporting Information: **4chloro123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -701.812761511 Predicted Change= -1.329606D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00077	0.00180	[YES]	0.00077	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.594780	1.102093	0.000051
C	0.248913	0.012833	-0.000018
N	-1.821740	0.526064	0.000110
H	-2.731218	0.967993	0.000178
H	-0.423623	2.166417	0.000054
N	-1.745961	-0.821011	0.000020
Cl	1.973493	0.010591	-0.000103
N	-0.477918	-1.134197	0.000059

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -701.812761511 Predicted Change= -1.329606D-07

Zero-point correction (ZPE)= -701.7630 0.04969

Internal Energy (U)= -701.7584 0.05430

Enthalpy (H)= -701.7575 0.05525

Gibbs Free Energy (G)= -701.7916 0.02108

Frequencies -- 258.2825 313.3851 492.5981

Supporting Information: **4radical123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -241.523484070 Predicted Change= -1.655325D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005 ‖	0.00045	[YES]	0.00001 ‖	0.00030	[YES]
Displ	0.00025 ‖	0.00180	[YES]	0.00025 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.589342	1.104579	0.000049
C	0.233598	0.001316	0.000011
N	-1.821276	0.527507	0.000102
H	-2.733172	0.966214	0.000152
H	-0.421978	2.169083	0.000060
N	-1.750895	-0.822176	0.000089
N	-0.463261	-1.126331	-0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -241.523484070 Predicted Change= -1.655325D-08
Zero-point correction (ZPE)= -241.4772 0.04626
Internal Energy (U)= -241.4736 0.04983
Enthalpy (H)= -241.4727 0.05077
Gibbs Free Energy (G)= -241.5039 0.01953

Frequencies -- 582.8429 612.7180 713.7587

Supporting Information: **5chloro123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -701.810521244 Predicted Change= -8.543099D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013 ‖	0.00045	[YES]	0.00004 ‖	0.00030	[YES]
Displ	0.00048 ‖	0.00180	[YES]	0.00048 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.241480	0.081935	0.000002
C	-0.646176	1.133456	0.000090
N	-0.544276	-1.023093	-0.000067
H	-0.268349	-1.996074	-0.000128
H	-0.450127	2.194757	0.000169
N	-1.853252	-0.684487	0.000017
Cl	1.958387	0.007127	0.000021
N	-1.909034	0.620125	-0.000086

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -701.810521244 Predicted Change= -8.543099D-08
Zero-point correction (ZPE)= -701.7608 0.04969
Internal Energy (U)= -701.7561 0.05434
Enthalpy (H)= -701.7552 0.05529
Gibbs Free Energy (G)= -701.7895 0.02101

Frequencies -- 243.6613 293.3372 491.4317

Supporting Information: **5radical123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -241.521030278 Predicted Change= -2.419596D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00047	0.00180	[YES]	0.00047	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.223568	0.077537	-0.000023
C	-0.639343	1.144751	0.000040
N	-0.539342	-1.029781	-0.000021
H	-0.266774	-2.002588	-0.000062
H	-0.451005	2.206064	0.000140
N	-1.854496	-0.691154	-0.000220
N	-1.902342	0.621790	0.000143

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -241.521030278 Predicted Change= -2.419596D-07
Zero-point correction (ZPE)= -241.4748 0.04619
Internal Energy (U)= -241.4712 0.04978
Enthalpy (H)= -241.4702 0.05073
Gibbs Free Energy (G)= -241.5015 0.01943

Frequencies -- 507.8437 614.1568 719.8586

Chlorooxadiazoles

Supporting Information: **3chloro124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7

Charge = 0 Multiplicity = 1

SCF Energy= -721.675268212 Predicted Change= -5.549702D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00115	0.00180	[YES]	0.00115	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.733446	0.646300	0.000343
C	-0.218438	-0.003219	0.000657
H	2.676701	1.175679	0.000103
N	0.442972	-1.134101	-0.000219
O	1.779261	-0.690226	-0.000186
Cl	-1.932174	0.024801	-0.000021
N	0.535046	1.143534	-0.000390

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.675268212 Predicted Change= -5.549702D-07

Zero-point correction (ZPE)= -721.6381 0.03713

Internal Energy (U)= -721.6337 0.04153

Enthalpy (H)= -721.6327 0.04247

Gibbs Free Energy (G)= -721.6666 0.00865

Frequencies -- 261.7028 332.9190 504.8410

Supporting Information: **3radical124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -261.388229628 Predicted Change= -1.020114D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00031	0.00180	[YES]	0.00031	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.733448	0.644847	-0.000007
C	-0.191465	-0.001375	-0.000026
H	2.673024	1.181902	0.000024
N	0.411977	-1.140860	0.000142
O	1.794252	-0.689317	-0.000111
N	0.527753	1.142770	0.000286

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -261.388229628 Predicted Change= -1.020114D-07
Zero-point correction (ZPE)= -261.3548 0.03333
Internal Energy (U)= -261.3514 0.03678
Enthalpy (H)= -261.3504 0.03773
Gibbs Free Energy (G)= -261.3815 0.00664

Frequencies -- 593.1878 651.4483 693.2252

Supporting Information: **5chloro124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -721.674851833 Predicted Change= -2.554823D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.206234	0.092088	-0.000177
C	1.791335	0.586009	-0.000169
N	1.828490	-0.720857	0.000173
H	2.701850	1.170580	0.000014
O	0.458981	-1.068991	-0.000030
Cl	-1.909007	0.016741	-0.000056
N	0.538484	1.153453	0.000292

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.674851833 Predicted Change= -2.554823D-07
Zero-point correction (ZPE)= -721.6377 0.03713
Internal Energy (U)= -721.6333 0.04154
Enthalpy (H)= -721.6323 0.04249
Gibbs Free Energy (G)= -721.6662 0.00864

Frequencies -- 245.0276 327.3838 511.0732

Supporting Information: **5radical124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -261.387643287 Predicted Change= -2.951091D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00048	0.00180	[YES]	0.00048	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.181831	0.089548	0.000000
C	1.791897	0.586184	0.000070
N	1.840138	-0.720461	-0.000018
H	2.701196	1.173351	0.000060
O	0.433442	-1.071689	-0.000015
N	0.528063	1.155350	0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -261.387643287 Predicted Change= -2.951091D-07
Zero-point correction (ZPE)= -261.3542 0.03338
Internal Energy (U)= -261.3508 0.03683
Enthalpy (H)= -261.3498 0.03778
Gibbs Free Energy (G)= -261.3809 0.00669

Frequencies -- 599.1916 633.6765 719.1701

Supporting Information: **3chloro125oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -721.634651985 Predicted Change= -3.693500D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00021	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00150	0.00180	[YES]	0.00150	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.645557	1.106772	0.000008
C	-0.238899	-0.011300	-0.000068
H	0.419660	2.163179	0.000065
N	0.452670	-1.119592	0.000177
O	1.762246	-0.710507	-0.000265
Cl	-1.954290	0.009218	0.000015
N	1.870952	0.661212	0.000132

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.634651985 Predicted Change= -3.693500D-07
Zero-point correction (ZPE)= -721.5982 0.03640
Internal Energy (U)= -721.5937 0.04088
Enthalpy (H)= -721.5928 0.04182
Gibbs Free Energy (G)= -721.6268 0.00784

Frequencies -- 266.1600 308.9123 495.9116

Supporting Information: **3radical125oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -261.347451574 Predicted Change= -6.971327D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00131	0.00180	[YES]	0.00131	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.642812	1.113947	-0.000022
C	-0.218338	-0.020916	0.000264
H	0.417006	2.169345	0.000075
N	0.427443	-1.124452	-0.000325
O	1.774068	-0.712508	0.000222
N	1.869196	0.664348	-0.000165

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -261.347451574 Predicted Change= -6.971327D-07
Zero-point correction (ZPE)= -261.3148 0.03261
Internal Energy (U)= -261.3113 0.03611
Enthalpy (H)= -261.3103 0.03706
Gibbs Free Energy (G)= -261.3415 0.00588

Frequencies -- 590.8739 637.8888 718.4818

Supporting Information: **2chloro134oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -721.681290129 Predicted Change= -6.089758D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00167	0.00180	[YES]	0.00167	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.211887	0.095012	-0.000033
C	1.777614	-0.582860	0.000119
H	2.583853	-1.300493	0.000194
N	1.841079	0.705928	0.000100
O	0.501438	-1.061967	0.000075
Cl	-1.910338	-0.020859	-0.000120
N	0.514068	1.162345	0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.681290129 Predicted Change= -6.089758D-07
Zero-point correction (ZPE)= -721.6443 0.03697
Internal Energy (U)= -721.6398 0.04141
Enthalpy (H)= -721.6389 0.04235
Gibbs Free Energy (G)= -721.6728 0.00847

Frequencies -- 243.5391 326.5867 510.0762

Supporting Information: **2radical134oxadiazole.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C2HN2O(2)   C1[X(C2HN2O)]  #Atoms= 6
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -261.392045917     Predicted Change= -6.536987D-08
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00009 ||  0.00045   [ YES ]      0.00003 ||  0.00030   [ YES ]
 Displ      0.00032 ||  0.00180   [ YES ]      0.00032 ||  0.00180   [ YES ]
---------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
      Type       X           Y       Z
---------------------------------------------------------------------
      C       -0.190284       0.098100       0.000025
      C        1.777289      -0.586662       0.000248
      H        2.585735      -1.302197       0.000249
      N        1.846990       0.703032      -0.000078
      O        0.494386      -1.066193      -0.000077
      N        0.492049       1.171886       0.000092
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -261.392045917 Predicted Change= -6.536987D-08
 Zero-point correction (ZPE)=         -261.3588  0.03315
 Internal Energy (U)=                 -261.3554  0.03661
 Enthalpy (H)=                        -261.3544   0.03755
 Gibbs Free Energy (G)=               -261.3855    0.00646
---------------------------------------------------------------------
 Frequencies --   575.2518              641.4795              833.8866
```

Chlorotriazines

Supporting Information: **3chloro124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -739.915719149 Predicted Change= -6.458443D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00117	0.00180	[YES]	0.00117	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	0.140906	-1.192192	0.000086
C	-0.432775	0.012658	0.000224
C	1.490888	1.148428	0.000008
C	2.151469	-0.083995	-0.000006
N	1.475133	-1.233423	0.000010
H	2.030695	2.093254	-0.000006
H	3.234233	-0.164189	-0.000039
N	0.162492	1.204874	0.000088
Cl	-2.174831	0.009034	-0.000153

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -739.915719149 Predicted Change= -6.458443D-07

Zero-point correction (ZPE)= -739.8612 0.05446

Internal Energy (U)= -739.8560 0.05968

Enthalpy (H)= -739.8550 0.06062

Gibbs Free Energy (G)= -739.8909 0.02475

Frequencies -- 150.5453 326.4030 383.6515

Supporting Information: **3radical124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -279.638055941 Predicted Change= -9.508601D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00137	0.00180	[YES]	0.00137	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	0.123193	-1.190464	0.000121
C	-0.402133	0.009843	0.000152
C	1.490857	1.157176	0.000021
C	2.142768	-0.085764	-0.000012
N	1.479822	-1.240457	0.000035
H	2.035030	2.099312	0.000004
H	3.226851	-0.161605	-0.000070
N	0.156653	1.197375	0.000113

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -279.638055941 Predicted Change= -9.508601D-07
Zero-point correction (ZPE)= -279.5871 0.05088
Internal Energy (U)= -279.5829 0.05506
Enthalpy (H)= -279.5820 0.05601
Gibbs Free Energy (G)= -279.6151 0.02292

Frequencies -- 332.3374 372.4657 567.1194

Supporting Information: **5chloro124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -739.918965049 Predicted Change= -3.214709D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00059	0.00180	[YES]	0.00059	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.233427	0.014811	0.000013
C	1.507092	-1.101042	0.000019
C	-0.456399	-0.035631	-0.000012
C	0.250815	1.178227	0.000000
N	1.579589	1.182984	0.000008
H	2.063343	-2.034402	-0.000007
H	-0.248676	2.141875	0.000002
N	0.164722	-1.191845	-0.000004
Cl	-2.203993	-0.023438	-0.000009

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -739.918965049 Predicted Change= -3.214709D-07
Zero-point correction (ZPE)= -739.8642 0.05474
Internal Energy (U)= -739.8589 0.05996
Enthalpy (H)= -739.8580 0.06091
Gibbs Free Energy (G)= -739.8939 0.02500

Frequencies -- 158.3638 306.3030 379.8367

Supporting Information: **5radical124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -279.647127649 Predicted Change= -1.031448D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00039	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00098	0.00180	[YES]	0.00098	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.221485	0.013726	0.000011
C	1.521159	-1.116591	-0.000030
C	-0.454453	-0.039492	-0.000002
C	0.233344	1.184233	0.000003
N	1.570091	1.167868	0.000014
H	2.077248	-2.049043	0.000029
H	-0.245415	2.156907	0.000003
N	0.170454	-1.162630	-0.000009

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -279.647127649 Predicted Change= -1.031448D-06
Zero-point correction (ZPE)= -279.5956 0.05143
Internal Energy (U)= -279.5915 0.05557
Enthalpy (H)= -279.5906 0.05651
Gibbs Free Energy (G)= -279.6236 0.02350

Frequencies -- 324.9214 402.3258 596.8091

Supporting Information: **6chloro124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -739.915923353 Predicted Change= -3.574670D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00035	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00085	0.00180	[YES]	0.00085	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.495028	-1.213194	-0.000006
C	2.135933	-0.045337	-0.000004
C	0.258404	1.194713	0.000007
C	-0.449049	-0.019674	0.000001
N	0.155174	-1.195471	-0.000005
H	3.220633	-0.103319	0.000009
H	-0.254202	2.153935	0.000010
N	1.581825	1.179427	0.000007
Cl	-2.191903	-0.013186	-0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -739.915923353 Predicted Change= -3.574670D-07
Zero-point correction (ZPE)= -739.8612 0.05462
Internal Energy (U)= -739.8560 0.05986
Enthalpy (H)= -739.8551 0.06080
Gibbs Free Energy (G)= -739.8910 0.02490

Frequencies -- 164.8113 304.4661 391.9737

Supporting Information: **6radical124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -279.640386728 Predicted Change= -1.216984D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00041	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00152	0.00180	[YES]	0.00152	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.512968	-1.236981	-0.000003
C	2.132974	-0.056705	-0.000018
C	0.241001	1.200500	0.000015
C	-0.438138	-0.029517	0.000000
N	0.161449	-1.157785	-0.000005
H	3.219113	-0.100271	0.000017
H	-0.253956	2.167347	0.000008
N	1.568336	1.164492	0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -279.640386728 Predicted Change= -1.216984D-06
Zero-point correction (ZPE)= -279.5891 0.05119
Internal Energy (U)= -279.5850 0.05538
Enthalpy (H)= -279.5840 0.05632
Gibbs Free Energy (G)= -279.6171 0.02323

Frequencies -- 337.1451 378.1635 549.1041

Supporting Information: **2chloro135triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -739.960942391 Predicted Change= -4.730537D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00076	0.00180	[YES]	0.00076	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.491945	1.119086	0.000009
N	0.156328	1.189102	-0.000004
C	-0.437962	0.000077	-0.000022
C	1.492213	-1.118929	-0.000008
N	2.221755	-0.000166	0.000013
H	2.028608	2.065334	0.000013
H	2.028072	-2.065727	0.000014
N	0.156067	-1.189039	0.000000
Cl	-2.180759	-0.000017	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -739.960942391 Predicted Change= -4.730537D-07
Zero-point correction (ZPE)= -739.9051 0.05577
Internal Energy (U)= -739.9000 0.06090
Enthalpy (H)= -739.8990 0.06185
Gibbs Free Energy (G)= -739.9348 0.02611

Frequencies -- 155.0728 333.1212 365.9962

Supporting Information: **2radical135triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -279.684520285 Predicted Change= -2.411303D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00043	0.00180	[YES]	0.00043	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.491639	1.126348	-0.000002
N	0.146525	1.185006	-0.000006
C	-0.413335	0.000072	-0.000017
C	1.491530	-1.126431	0.000032
N	2.207257	-0.000139	0.000015
H	2.033744	2.069582	0.000013
H	2.033380	-2.069812	-0.000008
N	0.146286	-1.184888	-0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -279.684520285 Predicted Change= -2.411303D-07
Zero-point correction (ZPE)= -279.6322 0.05231
Internal Energy (U)= -279.6281 0.05640
Enthalpy (H)= -279.6271 0.05735
Gibbs Free Energy (G)= -279.6601 0.02441

Frequencies -- 326.7783 388.1746 643.2910

Chlorotriazoles

Supporting Information: **3chloro124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -701.840582235 Predicted Change= -5.505416D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00060	0.00180	[YES]	0.00060	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.738224	0.704206	0.000063
C	-0.225201	0.006226	0.000035
N	1.737549	-0.645831	-0.000045
H	2.512158	-1.294664	-0.000121
H	2.637665	1.304650	0.000106
Cl	-1.948386	0.000716	-0.000001
N	0.465771	-1.123382	-0.000076
N	0.495908	1.157104	0.000043

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -701.840582235 Predicted Change= -5.505416D-07

Zero-point correction (ZPE)= -701.7902 0.05037

Internal Energy (U)= -701.7856 0.05492

Enthalpy (H)= -701.7847 0.05587

Gibbs Free Energy (G)= -701.8187 0.02183

Frequencies -- 260.6474 336.3848 503.9055

Supporting Information: **3radical124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -241.551519047 Predicted Change= -1.358849D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00041	0.00180	[YES]	0.00041	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.737028	0.703889	0.000112
C	-0.206187	0.009566	0.000015
N	1.739570	-0.647626	-0.000087
H	2.517350	-1.293670	-0.000179
H	2.636829	1.304484	0.000152
N	0.450623	-1.123919	0.000024
N	0.486861	1.155585	-0.000031

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -241.551519047 Predicted Change= -1.358849D-07
Zero-point correction (ZPE)= -241.5047 0.04680
Internal Energy (U)= -241.5011 0.05036
Enthalpy (H)= -241.5002 0.05131
Gibbs Free Energy (G)= -241.5314 0.02008

Frequencies -- 517.6798 647.4229 672.1439

Supporting Information: **5chloro124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -701.840140515 Predicted Change= -7.426978D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037 ‖	0.00045	[YES]	0.00013 ‖	0.00030	[YES]
Displ	0.00075 ‖	0.00180	[YES]	0.00075 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.217301	-0.084068	0.000007
C	-1.792176	-0.629191	0.000064
N	-0.541794	1.033936	0.000054
H	-0.255388	2.002835	0.000105
N	-1.857101	0.694168	0.000046
H	-2.683707	-1.240715	0.000043
Cl	1.936253	-0.026379	-0.000032
N	-0.533671	-1.161551	-0.000104

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -701.840140515 Predicted Change= -7.426978D-07
Zero-point correction (ZPE)= -701.7896 0.05046
Internal Energy (U)= -701.7850 0.05505
Enthalpy (H)= -701.7841 0.05600
Gibbs Free Energy (G)= -701.8182 0.02187

Frequencies -- 248.5806 318.4569 500.2056

Supporting Information: **5radical124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -241.552729179 Predicted Change= -1.072279D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00043	0.00180	[YES]	0.00043	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.202976	-0.088516	0.000027
C	-1.795211	-0.629451	-0.000069
N	-0.533151	1.035371	0.000001
H	-0.250723	2.003688	-0.000007
N	-1.862597	0.693039	0.000321
H	-2.684508	-1.244361	-0.000057
N	-0.523323	-1.154356	-0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -241.552729179 Predicted Change= -1.072279D-07
Zero-point correction (ZPE)= -241.5057 0.04700
Internal Energy (U)= -241.5021 0.05060
Enthalpy (H)= -241.5011 0.05155
Gibbs Free Energy (G)= -241.5324 0.02024

Frequencies -- 457.4348 637.1000 683.9798

Chlorobenzofurans

Supporting Information: **2chlorobenzofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClO C1[X(C8H5ClO)] #Atoms= 15

Charge = 0 Multiplicity = 1

SCF Energy= -843.265351947 Predicted Change= -3.071535D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00193	0.00180	[NO]	0.00193	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.167717	-0.201099	-0.812291
C	-3.760008	-0.190642	-0.812379
C	-3.096646	1.045479	-0.812302
C	-3.863464	2.207649	-0.812144
C	-5.269631	2.159641	-0.812062
C	-5.952664	0.943210	-0.812133
C	-4.517329	-2.283589	-0.812588
C	-3.359316	-1.577895	-0.812538
H	-2.011550	1.094863	-0.812361
H	-3.367138	3.174040	-0.812081
H	-5.836034	3.086380	-0.811938
H	-7.035992	0.886710	-0.812067
H	-2.360209	-1.987796	-0.812637
O	-5.634204	-1.496441	-0.812369
Cl	-4.804897	-3.975745	-0.812787

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -843.265351947 Predicted Change= -3.071535D-07

Zero-point correction (ZPE)= -843.1573 0.10800

Internal Energy (U)= -843.1501 0.11518

Enthalpy (H)= -843.1492 0.11612

Gibbs Free Energy (G)= -843.1896 0.07565

Frequencies -- 113.5713 218.4535 251.2277

Supporting Information: **2radicalbenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5O(2) C1[X(C8H5O)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -382.975054744 Predicted Change= -1.159071D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00040	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00118	0.00180	[YES]	0.00118	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.169936	-0.197475	-0.812294
C	-3.761299	-0.191526	-0.812383
C	-3.097837	1.044073	-0.812304
C	-3.865093	2.206939	-0.812141
C	-5.271061	2.161527	-0.812057
C	-5.955296	0.945288	-0.812133
C	-4.522214	-2.261096	-0.812541
C	-3.350466	-1.588206	-0.812544
H	-2.012776	1.093795	-0.812367
H	-3.367369	3.172717	-0.812077
H	-5.836067	3.089082	-0.811931
H	-7.038663	0.888375	-0.812072
H	-2.351118	-1.995290	-0.812646
O	-5.632708	-1.507691	-0.812398

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -382.975054744 Predicted Change= -1.159071D-06
Zero-point correction (ZPE)= -382.8703 0.10469
Internal Energy (U)= -382.8644 0.11065
Enthalpy (H)= -382.8634 0.11159
Gibbs Free Energy (G)= -382.9011 0.07392

Frequencies -- 223.7730 252.4734 411.1021

Supporting Information: **3chlorobenzofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClO C1[X(C8H5ClO)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -843.264890254 Predicted Change= -2.327895D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00120	0.00180	[YES]	0.00120	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.173039	-0.197416	-0.812282
C	-3.766494	-0.179807	-0.812350
C	-3.093325	1.048964	-0.812278
C	-3.856216	2.212414	-0.812146
C	-5.263771	2.166701	-0.812084
C	-5.951053	0.954021	-0.812150
C	-4.535541	-2.298766	-0.812573
C	-3.390056	-1.571299	-0.812483
H	-2.008241	1.086218	-0.812322
H	-3.357946	3.177641	-0.812085
H	-5.826896	3.095484	-0.811977
H	-7.034726	0.902182	-0.812094
H	-4.723710	-3.361158	-0.812708
O	-5.640748	-1.486967	-0.812331
Cl	-1.774498	-2.197577	-0.812608

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -843.264890254 Predicted Change= -2.327895D-07
Zero-point correction (ZPE)= -843.1566 0.10823
Internal Energy (U)= -843.1494 0.11542
Enthalpy (H)= -843.1485 0.11637
Gibbs Free Energy (G)= -843.1890 0.07583

Frequencies -- 138.7812 175.2822 227.6539

Supporting Information: **3radicalbenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5O(2) C1[X(C8H5O)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -382.974471333 Predicted Change= -7.738949D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00096	0.00180	[YES]	0.00096	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.167676	-0.200769	-0.812305
C	-3.752845	-0.179270	-0.812376
C	-3.089224	1.056259	-0.812286
C	-3.855496	2.217082	-0.812128
C	-5.262741	2.167194	-0.812061
C	-5.944398	0.951674	-0.812150
C	-4.532884	-2.312017	-0.812507
C	-3.410823	-1.568971	-0.812537
H	-2.004420	1.100861	-0.812341
H	-3.360219	3.183909	-0.812059
H	-5.829195	3.093964	-0.811947
H	-7.028365	0.896043	-0.812111
H	-4.736398	-3.371012	-0.812611
O	-5.647081	-1.486734	-0.812445

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -382.974471333 Predicted Change= -7.738949D-07
Zero-point correction (ZPE)= -382.8694 0.10503
Internal Energy (U)= -382.8635 0.11096
Enthalpy (H)= -382.8625 0.11190
Gibbs Free Energy (G)= -382.9001 0.07429

Frequencies -- 219.4298 256.3079 417.6671

Supporting Information: **4chlorobenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClO C1[X(C8H5ClO)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -843.269425941 Predicted Change= -3.551721D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00166	0.00180	[YES]	0.00166	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.179308	-0.195502	-0.812285
C	-3.770125	-0.199634	-0.812397
C	-3.115301	1.038623	-0.812329
C	-3.856804	2.214061	-0.812162
C	-5.262728	2.166971	-0.812058
C	-5.954805	0.957485	-0.812116
C	-4.539379	-2.292454	-0.812597
C	-3.381892	-1.587106	-0.812560
H	-3.343304	3.169531	-0.812109
H	-5.817545	3.100436	-0.811926
H	-7.038252	0.910792	-0.812032
H	-4.750443	-3.351443	-0.812725
O	-5.647686	-1.481039	-0.812349
H	-2.378486	-1.986482	-0.812674
Cl	-1.359476	1.097022	-0.812456

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -843.269425941 Predicted Change= -3.551721D-07
Zero-point correction (ZPE)= -843.1613 0.10808
Internal Energy (U)= -843.1541 0.11526
Enthalpy (H)= -843.1532 0.11620
Gibbs Free Energy (G)= -843.1936 0.07576

Frequencies -- 155.2522 205.0585 222.8499

Supporting Information: **4radicalbenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5O(2) C1[X(C8H5O)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -382.984931868 Predicted Change= -4.340770D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00155	0.00180	[YES]	0.00155	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.174842	-0.198875	-0.812315
C	-3.759027	-0.204902	-0.812401
C	-3.156441	1.042050	-0.812301
C	-3.847861	2.228378	-0.812122
C	-5.263385	2.175894	-0.812047
C	-5.945262	0.960412	-0.812143
C	-4.538519	-2.298984	-0.812512
C	-3.378909	-1.597957	-0.812635
H	-3.339603	3.188646	-0.812055
H	-5.826979	3.105226	-0.811916
H	-7.028897	0.911216	-0.812087
H	-4.752796	-3.357361	-0.812567
O	-5.645463	-1.484333	-0.812424
H	-2.378074	-2.005171	-0.812796

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -382.984931868 Predicted Change= -4.340770D-07
Zero-point correction (ZPE)= -382.8801 0.10475
Internal Energy (U)= -382.8742 0.11068
Enthalpy (H)= -382.8733 0.11162
Gibbs Free Energy (G)= -382.9109 0.07401

Frequencies -- 212.6405 253.8622 410.0782

Supporting Information: **5chlorobenzofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClO C1[X(C8H5ClO)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -843.268684585 Predicted Change= -2.903001D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00045	0.00180	[YES]	0.00045	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.177630	-0.198232	-0.812344
C	-3.769820	-0.193207	-0.812425
C	-3.090995	1.034320	-0.812312
C	-3.859736	2.192016	-0.812116
C	-5.265798	2.170629	-0.812034
C	-5.949335	0.956756	-0.812152
C	-4.538433	-2.291890	-0.812428
C	-3.382421	-1.583597	-0.812640
H	-2.007889	1.088382	-0.812376
H	-5.812676	3.106763	-0.811897
H	-7.033277	0.914855	-0.812119
H	-4.746985	-3.351466	-0.812397
H	-2.380702	-1.989764	-0.812766
O	-5.648128	-1.483571	-0.812565
Cl	-3.045663	3.755961	-0.811982

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -843.268684585 Predicted Change= -2.903001D-08
Zero-point correction (ZPE)= -843.1606 0.10800
Internal Energy (U)= -843.1535 0.11518
Enthalpy (H)= -843.1525 0.11612
Gibbs Free Energy (G)= -843.1930 0.07567

Frequencies -- 124.3511 233.5373 240.7524

Supporting Information: **5radicalbenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5O(2) C1[X(C8H5O)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -382.985198679 Predicted Change= -3.854082D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00099	0.00180	[YES]	0.00099	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.171059	-0.191092	-0.812245
C	-3.760390	-0.194520	-0.812409
C	-3.076720	1.040923	-0.812430
C	-3.881959	2.153198	-0.812264
C	-5.270304	2.183495	-0.812104
C	-5.952895	0.959896	-0.812090
C	-4.540246	-2.289958	-0.812714
C	-3.380603	-1.587163	-0.812375
H	-1.991600	1.095797	-0.812487
H	-5.821049	3.119729	-0.811960
H	-7.037208	0.906214	-0.811955
H	-4.753405	-3.348764	-0.812926
H	-2.380884	-1.998516	-0.812357
O	-5.645503	-1.477245	-0.812254

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -382.985198679 Predicted Change= -3.854082D-07
Zero-point correction (ZPE)= -382.8806 0.10459
Internal Energy (U)= -382.8746 0.11053
Enthalpy (H)= -382.8737 0.11148
Gibbs Free Energy (G)= -382.9113 0.07387

Frequencies -- 222.3695 264.9698 410.0054

Supporting Information: **6radicalbenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5O(2) C1[X(C8H5O)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -382.985218969 Predicted Change= -3.873275D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00080	0.00180	[YES]	0.00080	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.186648	-0.198299	-0.812266
C	-3.775685	-0.187621	-0.812401
C	-3.095918	1.041048	-0.812365
C	-3.843901	2.223639	-0.812190
C	-5.227767	2.116198	-0.812057
C	-5.971014	0.958937	-0.812085
C	-4.539355	-2.291819	-0.812687
C	-3.387391	-1.579075	-0.812462
H	-2.009408	1.077705	-0.812437
H	-3.348650	3.190487	-0.812127
H	-7.055971	0.926284	-0.811975
H	-4.745837	-3.351738	-0.812875
O	-5.653087	-1.484749	-0.812337
H	-2.384601	-1.983163	-0.812496

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -382.985218969 Predicted Change= -3.873275D-07
Zero-point correction (ZPE)= -382.8806 0.10454
Internal Energy (U)= -382.8747 0.11049
Enthalpy (H)= -382.8737 0.11143
Gibbs Free Energy (G)= -382.9114 0.07381

Frequencies -- 225.8848 257.8600 411.2915

Supporting Information: **7chlorobenzofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClO C1[X(C8H5ClO)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -843.266363719 Predicted Change= -3.005008D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00173	0.00180	[YES]	0.00173	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.182719	-0.201746	-0.812277
C	-3.773667	-0.189535	-0.812393
C	-3.097526	1.039339	-0.812329
C	-3.852526	2.207819	-0.812155
C	-5.258824	2.179293	-0.812044
C	-5.940575	0.965472	-0.812104
C	-4.544512	-2.291030	-0.812587
C	-3.389734	-1.582217	-0.812562
H	-2.012340	1.078592	-0.812411
H	-3.351917	3.171747	-0.812100
H	-5.826775	3.103552	-0.811906
H	-4.756407	-3.349769	-0.812710
O	-5.654354	-1.480757	-0.812344
H	-2.387734	-1.987753	-0.812682
Cl	-7.687974	0.898359	-0.811961

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -843.266363719 Predicted Change= -3.005008D-07
Zero-point correction (ZPE)= -843.1582 0.10810
Internal Energy (U)= -843.1510 0.11528
Enthalpy (H)= -843.1501 0.11623
Gibbs Free Energy (G)= -843.1905 0.07577

Frequencies -- 150.6085 197.1316 218.5592

Supporting Information: **7radicalbenzofuran.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5O(2) C1[X(C8H5O)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -382.982408947 Predicted Change= -2.058169D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00070	0.00180	[YES]	0.00070	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.191731	-0.210007	-0.812308
C	-3.776524	-0.193834	-0.812404
C	-3.107034	1.041330	-0.812310
C	-3.853127	2.215605	-0.812128
C	-5.269951	2.191204	-0.812037
C	-5.898429	0.969439	-0.812133
C	-4.544864	-2.298250	-0.812522
C	-3.391573	-1.585985	-0.812620
H	-2.021508	1.080176	-0.812391
H	-3.345755	3.176853	-0.812065
H	-5.831808	3.121283	-0.811907
H	-4.749655	-3.358554	-0.812586
O	-5.658901	-1.495662	-0.812428
H	-2.388751	-1.990591	-0.812766

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -382.982408947 Predicted Change= -2.058169D-07
Zero-point correction (ZPE)= -382.8777 0.10470
Internal Energy (U)= -382.8717 0.11064
Enthalpy (H)= -382.8708 0.11159
Gibbs Free Energy (G)= -382.9084 0.07395

Frequencies -- 212.5453 255.0791 410.6018

Chlorobenzothiazoles

Supporting Information: **2chlorobenzothiazole2.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4ClNS C1[X(C7H4ClNS)] #Atoms= 14

Charge = 0 Multiplicity = 1

SCF Energy= -1182.29201379 Predicted Change= -4.642312D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00106	0.00180	[YES]	0.00106	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.360637	-0.129482	-0.812294
C	-3.947171	-0.221457	-0.812436
C	-3.176048	0.948385	-0.812366
C	-3.823390	2.178488	-0.812156
C	-5.226255	2.256491	-0.812015
C	-6.011065	1.105479	-0.812083
C	-4.385046	-2.368263	-0.812655
H	-2.093641	0.871495	-0.812475
H	-3.237302	3.092876	-0.812100
H	-5.709978	3.229071	-0.811850
H	-7.094638	1.171200	-0.811972
S	-6.044971	-1.749937	-0.812427
Cl	-4.132964	-4.081631	-0.812885
N	-3.430020	-1.512511	-0.812641

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1182.29201379 Predicted Change= -4.642312D-07

Zero-point correction (ZPE)= -1182.1988 0.09318

Internal Energy (U)= -1182.1912 0.10074

Enthalpy (H)= -1182.1903 0.10169

Gibbs Free Energy (G)= -1182.2319 0.06008

Frequencies -- 108.5959 195.7178 208.9368

Supporting Information: **2radicalbenzothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4NS(2) C1[X(C7H4NS)] #Atoms= 13
Charge = 0 Multiplicity = 2

SCF Energy= -722.015613541 Predicted Change= -7.463634D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00036	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00118	0.00180	[YES]	0.00118	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.357643	-0.127561	-0.812294
C	-3.944345	-0.211574	-0.812436
C	-3.171150	0.953177	-0.812366
C	-3.822383	2.182885	-0.812155
C	-5.224856	2.258354	-0.812015
C	-6.009061	1.105639	-0.812082
C	-4.383490	-2.369756	-0.812656
H	-2.088527	0.878890	-0.812475
H	-3.238262	3.098566	-0.812098
H	-5.709421	3.230582	-0.811851
H	-7.092906	1.170767	-0.811973
S	-6.041520	-1.768905	-0.812428
N	-3.456597	-1.529227	-0.812641

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -722.015613541 Predicted Change= -7.463634D-07
Zero-point correction (ZPE)= -721.9255 0.09006
Internal Energy (U)= -721.9191 0.09643
Enthalpy (H)= -721.9182 0.09737
Gibbs Free Energy (G)= -721.9571 0.05846

Frequencies -- 193.1488 217.6680 349.7472

Supporting Information: **4chlorobenzothiazole2.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4ClNS C1[X(C7H4ClNS)] #Atoms= 14
Charge = 0 Multiplicity = 1

SCF Energy= -1182.29215070 Predicted Change= -5.893547D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00024	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00111	0.00180	[YES]	0.00111	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.341504	-0.130696	-0.812288
C	-3.926179	-0.220039	-0.812439
C	-3.181054	0.973179	-0.812376
C	-3.835737	2.198073	-0.812168
C	-5.238804	2.253633	-0.812021
C	-6.009574	1.095757	-0.812078
C	-4.359805	-2.374089	-0.812657
H	-3.251837	3.112108	-0.812115
H	-5.727791	3.223348	-0.811856
H	-7.093453	1.147032	-0.811965
S	-6.011760	-1.751790	-0.812422
N	-3.407139	-1.503043	-0.812606
H	-4.192589	-3.445783	-0.812804
Cl	-1.434949	0.912461	-0.812534

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1182.29215070 Predicted Change= -5.893547D-07
Zero-point correction (ZPE)= -1182.1989 0.09318
Internal Energy (U)= -1182.1914 0.10071
Enthalpy (H)= -1182.1904 0.10165
Gibbs Free Energy (G)= -1182.2320 0.06012

Frequencies -- 128.2568 200.8712 205.4153

Supporting Information: **4radicalbenzothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4NS(2) C1[X(C7H4NS)] #Atoms= 13
Charge = 0 Multiplicity = 2

SCF Energy= -722.009203812 Predicted Change= -3.865265D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00035	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00103	0.00180	[YES]	0.00103	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.339739	-0.135250	-0.812301
C	-3.918241	-0.229460	-0.812461
C	-3.231680	0.976079	-0.812385
C	-3.824819	2.210935	-0.812163
C	-5.238379	2.263455	-0.811999
C	-5.999901	1.098386	-0.812072
C	-4.356721	-2.383285	-0.812598
H	-3.241557	3.127651	-0.812114
H	-5.735709	3.229940	-0.811829
H	-7.084062	1.149699	-0.811966
S	-6.010894	-1.757157	-0.812496
N	-3.400020	-1.517308	-0.812667
H	-4.195505	-3.455995	-0.812744

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -722.009203812 Predicted Change= -3.865265D-07
Zero-point correction (ZPE)= -721.9194 0.08980
Internal Energy (U)= -721.9131 0.09608
Enthalpy (H)= -721.9121 0.09702
Gibbs Free Energy (G)= -721.9509 0.05825

Frequencies -- 195.2415 208.8934 354.2365

Supporting Information: **5chlorobenzothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4ClNS C1[X(C7H4ClNS)] #Atoms= 14
Charge = 0 Multiplicity = 1

SCF Energy= -1182.29421188 Predicted Change= -8.531035D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00168	0.00180	[YES]	0.00168	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.982451	0.623484	-0.000006
C	0.551901	-0.725721	0.000131
C	-0.818064	-1.025059	0.000066
C	-1.716322	0.031721	-0.000135
C	-1.293897	1.371571	-0.000277
C	0.063407	1.675583	-0.000212
C	2.719697	-1.099152	0.000342
H	-1.150469	-2.056458	0.000177
H	-2.032343	2.165692	-0.000441
H	0.389629	2.710695	-0.000328
S	2.735072	0.667754	0.000121
N	1.564372	-1.675431	0.000337
H	3.660444	-1.639241	0.000480
Cl	-3.442003	-0.308899	-0.000215

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1182.29421188 Predicted Change= -8.531035D-07
Zero-point correction (ZPE)= -1182.2011 0.09310
Internal Energy (U)= -1182.1935 0.10063
Enthalpy (H)= -1182.1926 0.10158
Gibbs Free Energy (G)= -1182.2342 0.05999

Frequencies -- 106.8017 211.1393 226.5540

Supporting Information: **5radicalbenzothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4NS(2) C1[X(C7H4NS)] #Atoms= 13
Charge = 0 Multiplicity = 2

SCF Energy= -722.011280519 Predicted Change= -2.342516D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.972765	0.618535	-0.000012
C	0.550786	-0.736586	0.000129
C	-0.828173	-1.037424	0.000065
C	-1.671533	0.042138	-0.000133
C	-1.305434	1.380172	-0.000274
C	0.061174	1.679551	-0.000213
C	2.721519	-1.097631	0.000359
H	-1.162139	-2.070539	0.000171
H	-2.042723	2.177904	-0.000432
H	0.398714	2.712150	-0.000324
S	2.726423	0.668814	0.000092
N	1.568913	-1.679633	0.000328
H	3.665586	-1.632012	0.000499

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -722.011280519 Predicted Change= -2.342516D-07
Zero-point correction (ZPE)= -721.9215 0.08969
Internal Energy (U)= -721.9153 0.09598
Enthalpy (H)= -721.9143 0.09692
Gibbs Free Energy (G)= -721.9531 0.05817

Frequencies -- 204.4027 215.0445 359.6273

Supporting Information: **6chlorobenzothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4ClNS C1[X(C7H4ClNS)] #Atoms= 14
Charge = 0 Multiplicity = 1

SCF Energy= -1182.29434812 Predicted Change= -7.343470D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00163	0.00180	[YES]	0.00163	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.664011	-0.444490	0.000053
C	-0.950942	0.942890	0.000199
C	0.105087	1.865092	0.000132
C	1.413671	1.402456	-0.000076
C	1.668352	0.020918	-0.000219
C	0.647728	-0.923833	-0.000160
C	-3.023948	0.205044	0.000429
H	-0.114034	2.927783	0.000235
H	2.245459	2.098208	-0.000133
H	0.874553	-1.983892	-0.000274
S	-2.168966	-1.343668	0.000197
N	-2.299090	1.272734	0.000365
H	-4.108593	0.212818	0.000580
Cl	3.336710	-0.533754	-0.000486

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1182.29434812 Predicted Change= -7.343470D-07
Zero-point correction (ZPE)= -1182.2012 0.09309
Internal Energy (U)= -1182.1937 0.10063
Enthalpy (H)= -1182.1927 0.10157
Gibbs Free Energy (G)= -1182.2343 0.05998

Frequencies -- 117.3319 196.7899 217.9304

Supporting Information: **6radicalbenzothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4NS(2) C1[X(C7H4NS)] #Atoms= 13
Charge = 0 Multiplicity = 2

SCF Energy= -722.011458576 Predicted Change= -2.211884D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00074	0.00180	[YES]	0.00074	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.663538	-0.455199	0.000062
C	-0.942783	0.936636	0.000220
C	0.107049	1.869586	0.000144
C	1.424864	1.410109	-0.000093
C	1.621917	0.037079	-0.000240
C	0.655831	-0.938859	-0.000178
C	-3.022315	0.208050	0.000357
H	-0.124642	2.930604	0.000266
H	2.257416	2.107612	-0.000158
H	0.885202	-2.000311	-0.000280
S	-2.175639	-1.345747	0.000291
N	-2.291139	1.270567	0.000430
H	-4.106957	0.221932	0.000507

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -722.011458576 Predicted Change= -2.211884D-07
Zero-point correction (ZPE)= -721.9217 0.08968
Internal Energy (U)= -721.9154 0.09597
Enthalpy (H)= -721.9145 0.09692
Gibbs Free Energy (G)= -721.9532 0.05816

Frequencies -- 193.8012 225.2964 358.0506

Supporting Information: **7chlorobenzothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4ClNS C1[X(C7H4ClNS)] #Atoms= 14
Charge = 0 Multiplicity = 1

SCF Energy= -1182.29375165 Predicted Change= -8.881371D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00114	0.00180	[YES]	0.00114	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.174585	-0.158599	0.000023
C	-1.092250	0.922571	0.000183
C	-0.621658	2.242735	0.000124
C	0.749363	2.464623	-0.000085
C	1.661526	1.396221	-0.000244
C	1.200383	0.084482	-0.000194
C	-2.543622	-0.731931	0.000408
H	-1.333366	3.061361	0.000232
H	1.132308	3.480730	-0.000136
H	2.729898	1.583857	-0.000410
S	-1.048646	-1.673251	0.000166
N	-2.430998	0.554234	0.000327
H	-3.496294	-1.250954	0.000561
Cl	2.334579	-1.253131	-0.000382

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1182.29375165 Predicted Change= -8.881371D-07
Zero-point correction (ZPE)= -1182.2005 0.09317
Internal Energy (U)= -1182.1930 0.10071
Enthalpy (H)= -1182.1920 0.10165
Gibbs Free Energy (G)= -1182.2336 0.06011

Frequencies -- 128.2319 183.8228 210.2085

Supporting Information: **7radicalbenzothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H4NS(2) C1[X(C7H4NS)] #Atoms= 13
Charge = 0 Multiplicity = 2

SCF Energy= -722.011809465 Predicted Change= -4.842035D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00035	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00109	0.00180	[YES]	0.00109	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.174527	-0.167669	0.000036
C	-1.096690	0.919749	0.000209
C	-0.614424	2.238342	0.000143
C	0.755997	2.467977	-0.000101
C	1.678618	1.394741	-0.000283
C	1.169996	0.119273	-0.000190
C	-2.550000	-0.738419	0.000293
H	-1.324912	3.058401	0.000277
H	1.132554	3.487519	-0.000154
H	2.747779	1.587466	-0.000460
S	-1.055211	-1.683523	0.000323
N	-2.433091	0.547092	0.000413
H	-3.504030	-1.254869	0.000446

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -722.011809465 Predicted Change= -4.842035D-07
Zero-point correction (ZPE)= -721.9219 0.08986
Internal Energy (U)= -721.9156 0.09614
Enthalpy (H)= -721.9147 0.09708
Gibbs Free Energy (G)= -721.9534 0.05832

Frequencies -- 193.6390 211.5853 357.8320

Chlorobenzothiophene

Supporting Information: **2chlorobenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClS C1[X(C8H5ClS)] #Atoms= 15

Charge = 0 Multiplicity = 1

SCF Energy= -1166.24399941 Predicted Change= -5.198142D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00033	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00111	0.00180	[YES]	0.00111	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.309446	-0.131994	-0.812291
C	-3.893499	-0.203451	-0.812386
C	-3.155624	0.994207	-0.812301
C	-3.823861	2.211218	-0.812126
C	-5.228892	2.260941	-0.812034
C	-5.983600	1.091985	-0.812115
C	-4.427752	-2.463019	-0.812601
C	-3.413791	-1.561659	-0.812566
H	-2.069447	0.959562	-0.812372
H	-3.255386	3.136942	-0.812060
H	-5.733770	3.222778	-0.811897
H	-7.068929	1.131518	-0.812044
H	-2.366278	-1.839085	-0.812661
S	-6.032203	-1.737351	-0.812422
Cl	-4.274324	-4.187828	-0.812799

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1166.24399941 Predicted Change= -5.198142D-07

Zero-point correction (ZPE)= -1166.1390 0.10491

Internal Energy (U)= -1166.1313 0.11268

Enthalpy (H)= -1166.1303 0.11362

Gibbs Free Energy (G)= -1166.1723 0.07165

Frequencies -- 104.8441 195.8184 199.5144

Supporting Information: **2radicalbenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5S(2) C1[X(C8H5S)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -705.958694787 Predicted Change= -5.037083D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00200	0.00180	[NO]	0.00200	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.308892	-0.130787	-0.812291
C	-3.891718	-0.203494	-0.812387
C	-3.155324	0.994259	-0.812301
C	-3.825049	2.211372	-0.812126
C	-5.229671	2.261520	-0.812034
C	-5.984057	1.091774	-0.812116
C	-4.441714	-2.429393	-0.812596
C	-3.404324	-1.573784	-0.812567
H	-2.069031	0.960775	-0.812372
H	-3.256367	3.137127	-0.812059
H	-5.734840	3.223287	-0.811897
H	-7.069548	1.130421	-0.812044
H	-2.355795	-1.848731	-0.812663
S	-6.036147	-1.751752	-0.812423

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.958694787 Predicted Change= -5.037083D-07
Zero-point correction (ZPE)= -705.8570 0.10165
Internal Energy (U)= -705.8505 0.10817
Enthalpy (H)= -705.8495 0.10912
Gibbs Free Energy (G)= -705.8887 0.06993

Frequencies -- 193.3826 205.2581 342.1364

Supporting Information: **3chlorobenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClS C1[X(C8H5ClS)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -1166.24732306 Predicted Change= -6.855157D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00147	0.00180	[YES]	0.00147	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.298365	-0.136248	-0.812293
C	-3.884262	-0.192957	-0.812361
C	-3.146829	1.003034	-0.812271
C	-3.822466	2.215111	-0.812119
C	-5.228802	2.257415	-0.812054
C	-5.977770	1.086191	-0.812139
C	-4.423068	-2.482919	-0.812569
C	-3.427676	-1.561432	-0.812522
H	-2.061773	0.966992	-0.812322
H	-3.259233	3.143897	-0.812049
H	-5.737884	3.217060	-0.811934
H	-7.063361	1.119284	-0.812088
H	-4.322255	-3.559219	-0.812683
S	-6.009914	-1.744896	-0.812424
Cl	-1.732602	-1.980679	-0.812641

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1166.24732306 Predicted Change= -6.855157D-07
Zero-point correction (ZPE)= -1166.1423 0.10498
Internal Energy (U)= -1166.1346 0.11272
Enthalpy (H)= -1166.1336 0.11366
Gibbs Free Energy (G)= -1166.1755 0.07177

Frequencies -- 132.4095 186.4073 202.9028

Supporting Information: **3radicalbenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5S(2) C1[X(C8H5S)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -705.961931561 Predicted Change= -1.089716D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00054	0.00180	[YES]	0.00054	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.298946	-0.136060	-0.812293
C	-3.877162	-0.189478	-0.812361
C	-3.142882	1.009170	-0.812272
C	-3.820654	2.220174	-0.812119
C	-5.227135	2.259434	-0.812053
C	-5.975917	1.087362	-0.812139
C	-4.405501	-2.503024	-0.812571
C	-3.460542	-1.555829	-0.812518
H	-2.057390	0.976608	-0.812322
H	-3.259796	3.150468	-0.812049
H	-5.737394	3.218540	-0.811932
H	-7.061812	1.121893	-0.812088
H	-4.322388	-3.580961	-0.812685
S	-6.016137	-1.746983	-0.812427

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.961931561 Predicted Change= -1.089716D-07
Zero-point correction (ZPE)= -705.8602 0.10167
Internal Energy (U)= -705.8537 0.10817
Enthalpy (H)= -705.8528 0.10911
Gibbs Free Energy (G)= -705.8919 0.06999

Frequencies -- 196.7214 202.5773 346.8577

Supporting Information: **4chlorobenzothiophene.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClS C1[X(C8H5ClS)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -1166.24927406 Predicted Change= -5.033971D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00033	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00104	0.00180	[YES]	0.00104	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.001907	0.650388	0.000061
C	0.007478	-0.347248	-0.000041
C	1.346668	0.085409	0.000038
C	1.662028	1.435092	0.000209
C	0.635242	2.394965	0.000307
C	-0.701552	2.015951	0.000235
C	-1.898273	-1.683878	-0.000241
C	-0.540772	-1.677898	-0.000220
H	2.701889	1.743211	0.000266
H	0.897370	3.448903	0.000441
H	-1.491225	2.760964	0.000312
H	0.067443	-2.574126	-0.000321
S	-2.599262	-0.079540	-0.000058
H	-2.553363	-2.545243	-0.000358
Cl	2.641919	-1.105750	-0.000088

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1166.24927406 Predicted Change= -5.033971D-07
Zero-point correction (ZPE)= -1166.1444 0.10484
Internal Energy (U)= -1166.1367 0.11254
Enthalpy (H)= -1166.1357 0.11349
Gibbs Free Energy (G)= -1166.1775 0.07168

Frequencies -- 128.7169 202.4584 203.8995

Supporting Information: **4radicalbenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5S(2) C1[X(C8H5S)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -705.965841039 Predicted Change= -2.158270D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00077	0.00180	[YES]	0.00077	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.005311	0.648713	0.000063
C	0.006721	-0.355584	-0.000042
C	1.312179	0.117392	0.000039
C	1.678139	1.436790	0.000207
C	0.641972	2.401445	0.000307
C	-0.693875	2.014092	0.000236
C	-1.900939	-1.692053	-0.000247
C	-0.543781	-1.687256	-0.000215
H	2.719292	1.747602	0.000265
H	0.896479	3.458317	0.000442
H	-1.482501	2.760581	0.000314
H	0.064450	-2.584377	-0.000315
S	-2.603445	-0.086403	-0.000054
H	-2.557617	-2.552308	-0.000369

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.965841039 Predicted Change= -2.158270D-07
Zero-point correction (ZPE)= -705.8643 0.10145
Internal Energy (U)= -705.8579 0.10792
Enthalpy (H)= -705.8569 0.10886
Gibbs Free Energy (G)= -705.8960 0.06981

Frequencies -- 196.3696 200.3848 344.0993

Supporting Information: **5chlorobenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClS C1[X(C8H5ClS)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -1166.24906948 Predicted Change= -9.093463D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00041	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00188	0.00180	[NO]	0.00188	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.964328	0.606263	0.000013
C	0.536833	-0.744855	0.000112
C	-0.841431	-1.028023	0.000038
C	-1.736948	0.029019	-0.000131
C	-1.311645	1.368685	-0.000229
C	0.046603	1.661383	-0.000157
C	2.850846	-1.031227	0.000314
C	1.648345	-1.661586	0.000279
H	-1.197595	-2.052829	0.000109
H	-2.047207	2.165413	-0.000360
H	0.380976	2.694508	-0.000232
H	1.536358	-2.740414	0.000373
S	2.716718	0.715568	0.000134
H	3.833987	-1.483632	0.000432
Cl	-3.465622	-0.307653	-0.000229

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1166.24906948 Predicted Change= -9.093463D-07
Zero-point correction (ZPE)= -1166.1443 0.10473
Internal Energy (U)= -1166.1366 0.11245
Enthalpy (H)= -1166.1356 0.11339
Gibbs Free Energy (G)= -1166.1775 0.07151

Frequencies -- 105.7704 201.9256 222.5243

Supporting Information: **5radicalbenzothiophene.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5S(2) C1[X(C8H5S)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -705.965519954 Predicted Change= -1.876837D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00064	0.00180	[YES]	0.00064	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.954441	0.602030	0.000014
C	0.535179	-0.754500	0.000113
C	-0.852140	-1.039590	0.000036
C	-1.694340	0.039668	-0.000131
C	-1.323506	1.377146	-0.000232
C	0.044124	1.665747	-0.000157
C	2.851567	-1.029313	0.000309
C	1.651648	-1.664974	0.000285
H	-1.209595	-2.066251	0.000108
H	-2.056864	2.178520	-0.000363
H	0.389216	2.696387	-0.000230
H	1.543844	-2.744361	0.000381
S	2.709881	0.715355	0.000139
H	3.836713	-1.477591	0.000422

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.965519954 Predicted Change= -1.876837D-07
Zero-point correction (ZPE)= -705.8641 0.10132
Internal Energy (U)= -705.8577 0.10779
Enthalpy (H)= -705.8567 0.10874
Gibbs Free Energy (G)= -705.8958 0.06969

Frequencies -- 198.5009 211.8112 347.9077

Supporting Information: **6chlorobenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClS C1[X(C8H5ClS)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -1166.24897996 Predicted Change= -7.455020D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037 ‖	0.00045	[YES]	0.00006 ‖	0.00030	[YES]
Displ	0.00165 ‖	0.00180	[YES]	0.00165 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.656694	-0.417282	0.000058
C	-0.941935	0.971161	0.000158
C	0.132819	1.879004	0.000074
C	1.438365	1.411460	-0.000102
C	1.683175	0.027319	-0.000197
C	0.653943	-0.904668	-0.000120
C	-3.102977	0.093652	0.000372
C	-2.359148	1.229073	0.000332
H	-0.059528	2.948456	0.000146
H	2.274908	2.101622	-0.000170
H	0.868943	-1.967643	-0.000196
H	-2.786976	2.225873	0.000427
S	-2.133397	-1.367181	0.000188
H	-4.181783	0.008381	0.000497
Cl	3.349029	-0.540006	-0.000421

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1166.24897996 Predicted Change= -7.455020D-07
Zero-point correction (ZPE)= -1166.1442 0.10471
Internal Energy (U)= -1166.1365 0.11243
Enthalpy (H)= -1166.1356 0.11337
Gibbs Free Energy (G)= -1166.1774 0.07149

Frequencies -- 114.9042 197.5353 212.6795

Supporting Information: **6radicalbenzothiophene.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5S(2) C1[X(C8H5S)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -705.965631384 Predicted Change= -1.471136D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.656396	-0.428412	0.000059
C	-0.934491	0.964303	0.000157
C	0.133189	1.883093	0.000073
C	1.448652	1.419089	-0.000105
C	1.638284	0.044431	-0.000192
C	0.662020	-0.919185	-0.000122
C	-3.102928	0.095817	0.000367
C	-2.352298	1.226080	0.000337
H	-0.070759	2.951487	0.000147
H	2.284159	2.113286	-0.000172
H	0.879483	-1.983642	-0.000197
H	-2.774942	2.225284	0.000433
S	-2.141918	-1.370190	0.000195
H	-4.182341	0.017787	0.000488

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.965631384 Predicted Change= -1.471136D-07
Zero-point correction (ZPE)= -705.8643 0.10128
Internal Energy (U)= -705.8578 0.10776
Enthalpy (H)= -705.8569 0.10870
Gibbs Free Energy (G)= -705.8959 0.06964

Frequencies -- 194.3851 214.1909 347.8857

Supporting Information: **7chlorobenzothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClS C1[X(C8H5ClS)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -1166.24843852 Predicted Change= -2.494259D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.179153	-0.130342	0.000025
C	-1.065617	0.977660	0.000135
C	-0.537639	2.281185	0.000061
C	0.837923	2.462107	-0.000118
C	1.714799	1.363274	-0.000228
C	1.204100	0.072149	-0.000155
C	-2.577040	-0.798938	0.000336
C	-2.442164	0.551608	0.000308
H	-1.207638	3.136361	0.000143
H	1.253232	3.465668	-0.000178
H	2.789065	1.513288	-0.000368
H	-3.280553	1.239884	0.000410
S	-1.047106	-1.652585	0.000143
H	-3.495667	-1.371242	0.000456
Cl	2.292000	-1.306754	-0.000291

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1166.24843852 Predicted Change= -2.494259D-07
Zero-point correction (ZPE)= -1166.1436 0.10477
Internal Energy (U)= -1166.1359 0.11249
Enthalpy (H)= -1166.1349 0.11344
Gibbs Free Energy (G)= -1166.1768 0.07162

Frequencies -- 127.6515 182.5035 202.9564

Supporting Information: **7radicalbenzothiophene.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5S(2) C1[X(C8H5S)] #Atoms= 14
Charge = 0 Multiplicity = 2

SCF Energy= -705.965532267 Predicted Change= -1.899172D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.179243	-0.138082	0.000027
C	-1.069963	0.975609	0.000136
C	-0.530180	2.276767	0.000059
C	0.845508	2.465238	-0.000121
C	1.732206	1.361115	-0.000231
C	1.175755	0.107543	-0.000151
C	-2.582494	-0.804400	0.000331
C	-2.445684	0.546389	0.000314
H	-1.198538	3.133656	0.000142
H	1.254402	3.472454	-0.000180
H	2.807614	1.515760	-0.000372
H	-3.285459	1.233469	0.000417
S	-1.054345	-1.661737	0.000152
H	-3.503036	-1.373705	0.000447

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.965532267 Predicted Change= -1.899172D-07
Zero-point correction (ZPE)= -705.8640 0.10145
Internal Energy (U)= -705.8576 0.10791
Enthalpy (H)= -705.8566 0.10885
Gibbs Free Energy (G)= -705.8957 0.06980

Frequencies -- 195.1892 202.6016 346.7274

Chloroimidazoles

Supporting Information: **24dichloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2Cl2N2 C1[X(C3H2Cl2N2)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -1145.39992279 Predicted Change= -5.543487D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00110	0.00180	[YES]	0.00110	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.029364	0.001781	0.000019
C	-1.079545	0.083520	0.000012
C	-0.677501	1.394487	0.000208
N	0.705293	1.324729	0.000019
H	1.354419	2.098827	0.000039
H	-1.218806	2.326852	0.000341
N	-0.017893	-0.781288	-0.000070
Cl	2.676570	-0.511257	-0.000056
Cl	-2.710766	-0.495125	-0.000029

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1145.39992279 Predicted Change= -5.543487D-07

Zero-point correction (ZPE)= -1145.3476 0.05224

Internal Energy (U)= -1145.3417 0.05820

Enthalpy (H)= -1145.3407 0.05914

Gibbs Free Energy (G)= -1145.3786 0.02123

Frequencies -- 162.2059 207.0135 295.3928

Supporting Information: **25dichloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2Cl2N2 C1[X(C3H2Cl2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1145.39747870 Predicted Change= -7.704615D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00051	0.00180	[YES]	0.00051	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.084466	0.160222	0.000073
C	-0.625245	1.436291	0.000085
C	-1.104952	0.153864	-0.000082
N	0.002336	-0.673286	0.000065
H	0.004827	-1.683621	0.000030
H	-1.185166	2.359973	0.000116
N	0.755959	1.422189	0.000152
Cl	2.689212	-0.477148	0.000139
Cl	-2.704114	-0.488789	-0.000263

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1145.39747870 Predicted Change= -7.704615D-08
Zero-point correction (ZPE)= -1145.3451 0.05231
Internal Energy (U)= -1145.3391 0.05831
Enthalpy (H)= -1145.3382 0.05926
Gibbs Free Energy (G)= -1145.3762 0.02122

Frequencies -- 154.8818 197.3596 286.1680

Supporting Information: **2chloro4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -685.112122251 Predicted Change= -2.746842D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ‖	0.00045	[YES]	0.00004 ‖	0.00030	[YES]
Displ	0.00126 ‖	0.00180	[YES]	0.00126 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.030728	0.002085	0.000285
C	-1.062154	0.079164	-0.000298
C	-0.687404	1.394223	0.000539
N	0.705236	1.325044	-0.000327
H	1.360042	2.095521	-0.000550
H	-1.223726	2.328942	0.000865
N	-0.030050	-0.775276	-0.000433
Cl	2.679229	-0.512052	0.000430

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.112122251 Predicted Change= -2.746842D-07
Zero-point correction (ZPE)= -685.0629 0.04913
Internal Energy (U)= -685.0582 0.05391
Enthalpy (H)= -685.0572 0.05485
Gibbs Free Energy (G)= -685.0922 0.01984

Frequencies -- 234.0516 324.2905 492.7059

Supporting Information: **2chloro5radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -685.107949099 Predicted Change= -4.750598D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00034	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00123	0.00180	[YES]	0.00123	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.084430	0.149573	0.000157
C	-0.637882	1.444921	0.000093
C	-1.088546	0.157775	0.000085
N	0.000686	-0.681717	0.000004
H	0.000496	-1.691238	-0.000077
H	-1.185760	2.373904	0.000097
N	0.750915	1.413035	0.000015
Cl	2.697099	-0.467770	0.000204

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.107949099 Predicted Change= -4.750598D-07
Zero-point correction (ZPE)= -685.0589 0.04897
Internal Energy (U)= -685.0541 0.05383
Enthalpy (H)= -685.0531 0.05478
Gibbs Free Energy (G)= -685.0883 0.01960

Frequencies -- 223.8663 320.0696 420.1323

Supporting Information: **2chloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -685.807434578 Predicted Change= -2.332688D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00123	0.00180	[YES]	0.00123	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.224293	-0.087193	-0.000032
C	-1.804522	-0.717410	0.000072
C	-1.847508	0.652692	0.000126
N	-0.523480	1.054059	0.000125
H	-0.168646	1.999253	0.000264
H	-2.632900	-1.412040	0.000077
H	-2.660483	1.362749	0.000194
N	-0.499749	-1.172474	-0.000033
Cl	1.952415	-0.012329	-0.000128

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.807434578 Predicted Change= -2.332688D-07
Zero-point correction (ZPE)= -685.7456 0.06178
Internal Energy (U)= -685.7408 0.06660
Enthalpy (H)= -685.7398 0.06755
Gibbs Free Energy (G)= -685.7743 0.03307

Frequencies -- 233.0405 320.1598 492.2723

Supporting Information: **2chloroimidazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.520336734 Predicted Change= -6.327915D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00036	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00080	0.00180	[YES]	0.00080	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.215508	-0.092113	0.000208
C	-1.812155	-0.718422	-0.000101
C	-1.849996	0.651410	0.000365
N	-0.514540	1.054200	-0.000038
H	-0.162477	1.999262	-0.000112
H	-2.636678	-1.417606	-0.000281
H	-2.663935	1.361498	0.000527
N	-0.488722	-1.158592	0.000224

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.520336734 Predicted Change= -6.327915D-07
Zero-point correction (ZPE)= -225.4620 0.05827
Internal Energy (U)= -225.4582 0.06212
Enthalpy (H)= -225.4572 0.06306
Gibbs Free Energy (G)= -225.4889 0.03137

Frequencies -- 418.9965 582.9750 625.1026

Supporting Information: **45dichloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2Cl2N2 C1[X(C3H2Cl2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1145.39741218 Predicted Change= -2.389251D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00119	0.00180	[YES]	0.00119	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.127049	2.195841	0.000470
C	-0.700696	0.231168	0.000095
C	0.663236	0.059378	0.000021
N	1.187310	1.335461	-0.000184
H	2.171593	1.564952	-0.000313
N	-1.023712	1.556865	-0.000492
Cl	1.657406	-1.340680	0.000002
H	0.250679	3.269895	0.000652
Cl	-1.898877	-1.012229	0.000049

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1145.39741218 Predicted Change= -2.389251D-07
Zero-point correction (ZPE)= -1145.3449 0.05247
Internal Energy (U)= -1145.3389 0.05844
Enthalpy (H)= -1145.3380 0.05938
Gibbs Free Energy (G)= -1145.3760 0.02140

Frequencies -- 166.4763 202.2684 258.2555

Supporting Information: **4chloro2radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -685.113401751 Predicted Change= -1.204715D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.017138	0.001100	-0.000233
C	-1.085076	0.084339	0.000173
C	-0.679990	1.394212	-0.000081
N	0.713386	1.322528	0.000269
H	1.360117	2.097092	0.000499
H	-1.223329	2.326252	-0.000069
N	-0.002941	-0.775457	-0.000385
Cl	-2.714739	-0.496285	0.000366

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.113401751 Predicted Change= -1.204715D-07
Zero-point correction (ZPE)= -685.0644 0.04890
Internal Energy (U)= -685.0596 0.05377
Enthalpy (H)= -685.0586 0.05471
Gibbs Free Energy (G)= -685.0938 0.01955

Frequencies -- 248.7898 320.3459 415.4843

Supporting Information: **4chloro5radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -685.106479004 Predicted Change= -3.779683D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00035	0.00180	[YES]	0.00035	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.134271	2.199178	0.000191
C	-0.703432	0.215789	-0.000013
C	0.654976	0.075355	-0.000154
N	1.194424	1.336959	-0.000045
H	2.178041	1.565959	-0.000111
N	-1.015240	1.550608	0.000176
H	0.245286	3.274743	0.000336
Cl	-1.911743	-1.017262	-0.000081

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.106479004 Predicted Change= -3.779683D-08
Zero-point correction (ZPE)= -685.0575 0.04897
Internal Energy (U)= -685.0526 0.05385
Enthalpy (H)= -685.0516 0.05479
Gibbs Free Energy (G)= -685.0869 0.01957

Frequencies -- 220.7982 322.5313 401.3830

Supporting Information: **4chloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -685.808586309 Predicted Change= -2.266710D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00119	0.00180	[YES]	0.00119	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.724542	-0.763293	-0.000088
C	-0.254940	0.002756	0.000017
C	0.551919	1.113817	0.000047
N	1.832209	0.597351	0.000065
H	2.688278	1.133290	0.000206
H	2.586438	-1.416390	-0.000155
H	0.339688	2.170853	0.000102
N	0.466791	-1.155053	-0.000125
Cl	-1.990384	-0.006089	0.000024

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.808586309 Predicted Change= -2.266710D-07
Zero-point correction (ZPE)= -685.7467 0.06186
Internal Energy (U)= -685.7419 0.06666
Enthalpy (H)= -685.7409 0.06761
Gibbs Free Energy (G)= -685.7754 0.03316

Frequencies -- 249.3284 317.1710 483.8614

Supporting Information: **4chloroimidazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.520044667 Predicted Change= -4.667938D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00136	0.00180	[YES]	0.00136	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.727395	-0.763739	0.000108
C	-0.243189	-0.006836	-0.000284
C	0.541865	1.115394	0.000255
N	1.832823	0.597060	-0.000159
H	2.692689	1.128760	-0.000181
H	2.588798	-1.417859	0.000191
H	0.336698	2.173475	0.000453
N	0.457846	-1.142924	-0.000313

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.520044667 Predicted Change= -4.667938D-07
Zero-point correction (ZPE)= -225.4614 0.05856
Internal Energy (U)= -225.4577 0.06230
Enthalpy (H)= -225.4567 0.06325
Gibbs Free Energy (G)= -225.4883 0.03173

Frequencies -- 523.4113 599.8841 671.1499

Supporting Information: **5chloro2radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -685.111951454 Predicted Change= -1.928187D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00097	0.00180	[YES]	0.00097	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.078168	0.167214	-0.000209
C	-0.632966	1.440709	0.000327
C	-1.105517	0.155464	-0.000320
N	0.011734	-0.676696	0.000283
H	0.011549	-1.685921	0.000478
H	-1.188536	2.366823	0.000570
N	0.759965	1.403635	-0.000296
Cl	-2.706286	-0.484385	-0.000656

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.111951454 Predicted Change= -1.928187D-07
Zero-point correction (ZPE)= -685.0629 0.04895
Internal Energy (U)= -685.0580 0.05386
Enthalpy (H)= -685.0571 0.05481
Gibbs Free Energy (G)= -685.0924 0.01952

Frequencies -- 230.3119 300.6384 400.7600

Supporting Information: **5chloro4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -685.109339716 Predicted Change= -1.927668D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00095	0.00180	[YES]	0.00095	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.128609	2.199392	0.000173
C	-0.697047	0.247001	-0.000270
C	0.656342	0.052992	0.000020
N	1.187216	1.336098	-0.000039
H	2.171214	1.570588	-0.000066
N	-1.019913	1.539962	0.000182
Cl	1.656910	-1.347044	-0.000095
H	0.249532	3.273889	0.000345

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.109339716 Predicted Change= -1.927668D-07
Zero-point correction (ZPE)= -685.0600 0.04931
Internal Energy (U)= -685.0552 0.05410
Enthalpy (H)= -685.0542 0.05504
Gibbs Free Energy (G)= -685.0893 0.01996

Frequencies -- 223.8103 305.7303 488.8453

Supporting Information: **5chloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -685.805641775 Predicted Change= -2.354376D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00196	0.00180	[NO]	0.00196	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.833526	-0.616490	0.000184
C	0.613868	1.150877	0.000077
C	-0.249931	0.086255	-0.000017
N	0.534302	-1.046853	-0.000006
H	0.196879	-1.998962	-0.000150
H	2.668082	-1.304663	0.000272
H	0.371364	2.203846	0.000093
N	1.913556	0.695607	0.000094
Cl	-1.973889	-0.009726	-0.000135

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.805641775 Predicted Change= -2.354376D-07
Zero-point correction (ZPE)= -685.7437 0.06190
Internal Energy (U)= -685.7388 0.06675
Enthalpy (H)= -685.7379 0.06769
Gibbs Free Energy (G)= -685.7725 0.03312

Frequencies -- 227.7795 297.5440 485.5308

Supporting Information: **5chloroimidazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.515272502 Predicted Change= -2.702695D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00124	0.00180	[YES]	0.00124	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.832216	-0.625756	0.000422
C	0.602928	1.163479	0.000179
C	-0.234662	0.084565	0.000232
N	0.532510	-1.053481	-0.000171
H	0.194121	-2.004418	-0.000355
H	2.675920	-1.302741	0.000539
H	0.374101	2.217817	0.000162
N	1.904513	0.690152	-0.000461

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.515272502 Predicted Change= -2.702695D-07
Zero-point correction (ZPE)= -225.4568 0.05843
Internal Energy (U)= -225.4530 0.06223
Enthalpy (H)= -225.4520 0.06317
Gibbs Free Energy (G)= -225.4837 0.03155

Frequencies -- 434.5255 556.1037 679.0587

Chloroindoles

Supporting Information: **2chloroindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6ClN C1[X(C8H6ClN)] #Atoms= 16

Charge = 0 Multiplicity = 1

SCF Energy= -823.410044554 Predicted Change= -1.736856D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00168	0.00180	[YES]	0.00168	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.583069	-0.655039	0.000133
C	-0.618064	0.768039	0.000061
C	-1.867497	1.412320	0.000156
C	-3.023398	0.642239	0.000310
C	-2.962544	-0.766015	0.000373
C	-1.743167	-1.434455	0.000288
C	1.525050	0.107686	-0.000201
C	0.743767	1.229728	-0.000086
H	-1.925384	2.497557	0.000116
H	-3.993547	1.131441	0.000389
H	-3.884338	-1.340980	0.000495
H	-1.695605	-2.520155	0.000342
H	1.097836	2.250153	-0.000160
N	0.747911	-1.032363	0.000033
H	1.107869	-1.974173	0.000054
Cl	3.248902	-0.037901	-0.000451

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -823.410044554 Predicted Change= -1.736856D-07

Zero-point correction (ZPE)= -823.2897 0.12027

Internal Energy (U)= -823.2821 0.12789

Enthalpy (H)= -823.2812 0.12884

Gibbs Free Energy (G)= -823.3224 0.08761

Frequencies -- 111.9603 214.1816 236.1486

Supporting Information: **2radicalindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6N(2) C1[X(C8H6N)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -363.118737995 Predicted Change= -1.831472D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00133	0.00180	[YES]	0.00133	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.584079	-0.658436	0.000139
C	-0.616475	0.765708	0.000064
C	-1.864948	1.411065	0.000153
C	-3.022199	0.641450	0.000311
C	-2.963889	-0.766326	0.000380
C	-1.744559	-1.436140	0.000295
C	1.504816	0.106768	-0.000122
C	0.752960	1.239469	-0.000096
H	-1.921679	2.496404	0.000102
H	-3.991656	1.132354	0.000383
H	-3.886541	-1.340032	0.000503
H	-1.697891	-2.522049	0.000347
H	1.095567	2.263391	-0.000177
N	0.755877	-1.037214	0.000020
H	1.110517	-1.980430	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -363.118737995 Predicted Change= -1.831472D-07
Zero-point correction (ZPE)= -363.0023 0.11637
Internal Energy (U)= -362.9955 0.12315
Enthalpy (H)= -362.9946 0.12410
Gibbs Free Energy (G)= -363.0345 0.08421

Frequencies -- 52.1130 235.4841 254.3743

Supporting Information: **3chloroindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6ClN C1[X(C8H6ClN)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -823.410015920 Predicted Change= -1.790552D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00095	0.00180	[YES]	0.00095	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.880954	0.910653	0.000058
C	0.076623	-0.262967	0.000000
C	0.696123	-1.523240	0.000086
C	2.082505	-1.584647	0.000221
C	2.865588	-0.410719	0.000271
C	2.279012	0.848623	0.000192
C	-1.280308	1.563424	-0.000307
C	-1.282506	0.193769	-0.000112
H	0.094785	-2.427688	0.000058
H	2.576599	-2.552153	0.000297
H	3.948946	-0.492439	0.000382
H	2.883764	1.751773	0.000238
H	-2.107211	2.257880	-0.000487
N	0.031563	1.999004	-0.000030
H	0.318853	2.965164	0.000001
Cl	-2.696742	-0.817938	-0.000161

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -823.410015920 Predicted Change= -1.790552D-07
Zero-point correction (ZPE)= -823.2895 0.12050
Internal Energy (U)= -823.2819 0.12811
Enthalpy (H)= -823.2809 0.12905
Gibbs Free Energy (G)= -823.3221 0.08786

Frequencies -- 139.6710 177.9220 221.1103

Supporting Information: **3radicalindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6N(2) C1[X(C8H6N)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -363.118147752 Predicted Change= -1.227097D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00087	0.00180	[YES]	0.00087	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.874904	0.909330	0.000044
C	0.068043	-0.274485	-0.000037
C	0.699419	-1.530598	0.000058
C	2.085707	-1.587465	0.000236
C	2.864777	-0.411039	0.000318
C	2.273028	0.845732	0.000224
C	-1.291624	1.567203	-0.000186
C	-1.271326	0.207363	-0.000186
H	0.104135	-2.439154	0.000001
H	2.583501	-2.553178	0.000310
H	3.948480	-0.488878	0.000442
H	2.875804	1.750816	0.000264
H	-2.110336	2.271708	-0.000289
N	0.031537	2.002694	-0.000149
H	0.329241	2.966389	-0.000182

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -363.118147752 Predicted Change= -1.227097D-07
Zero-point correction (ZPE)= -363.0010 0.11710
Internal Energy (U)= -362.9946 0.12350
Enthalpy (H)= -362.9936 0.12445
Gibbs Free Energy (G)= -363.0321 0.08603

Frequencies -- 205.1792 222.4355 330.8809

Supporting Information: **4chloroindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6ClN C1[X(C8H6ClN)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -823.413911542 Predicted Change= -1.576359D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00115 ‖	0.00180	[YES]	0.00115 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.325887	0.468304	0.000049
C	-0.216204	-0.425580	-0.000042
C	1.070015	0.136943	0.000028
C	1.240788	1.512496	0.000174
C	0.117082	2.363456	0.000255
C	-1.177261	1.859203	0.000194
C	-2.107620	-1.646673	-0.000386
C	-0.742605	-1.759005	-0.000144
H	2.242192	1.929207	0.000237
H	0.273772	3.438222	0.000378
H	-2.038657	2.521282	0.000268
H	-0.173628	-2.676996	-0.000183
N	-2.464170	-0.310784	-0.000016
H	-3.409101	0.040123	0.000047
H	-2.868304	-2.414776	-0.000603
Cl	2.474886	-0.924497	-0.000047

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -823.413911542 Predicted Change= -1.576359D-07
Zero-point correction (ZPE)= -823.2934 0.12044
Internal Energy (U)= -823.2859 0.12797
Enthalpy (H)= -823.2849 0.12891
Gibbs Free Energy (G)= -823.3259 0.08793

Frequencies -- 151.5895 205.6940 219.5741

Supporting Information: **4radicalindole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6N(2) C1[X(C8H6N)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -363.128887763 Predicted Change= -7.747849D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 ‖	0.00045	[YES]	0.00001 ‖	0.00030	[YES]
Displ	0.00093 ‖	0.00180	[YES]	0.00093 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.325475	0.463964	0.000065
C	-0.211234	-0.435846	-0.000114
C	1.040027	0.164522	-0.000069
C	1.256556	1.517206	0.000074
C	0.122366	2.370911	0.000262
C	-1.168421	1.856557	0.000265
C	-2.110834	-1.652073	-0.000545
C	-0.746756	-1.769158	0.000020
H	2.257040	1.941331	0.000127
H	0.270441	3.447906	0.000428
H	-2.031184	2.517531	0.000410
H	-0.183911	-2.691627	0.000151
N	-2.464520	-0.314301	-0.000021
H	-3.409749	0.036396	0.000058
H	-2.873935	-2.417897	-0.000855

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -363.128887763 Predicted Change= -7.747849D-08
Zero-point correction (ZPE)= -363.0118 0.11703
Internal Energy (U)= -363.0055 0.12333
Enthalpy (H)= -363.0046 0.12427
Gibbs Free Energy (G)= -363.0427 0.08609

Frequencies -- 208.5000 244.9270 374.0774

Supporting Information: **5chloroindole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6ClN C1[X(C8H6ClN)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -823.413095974 Predicted Change= -1.741906D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00124	0.00180	[YES]	0.00124	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.240404	0.684172	0.000020
C	0.864205	-0.689067	0.000105
C	-0.501316	-1.023625	0.000038
C	-1.426157	0.008371	-0.000102
C	-1.048966	1.365157	-0.000182
C	0.295573	1.714766	-0.000122
C	3.117032	-0.561520	0.000449
C	2.078722	-1.455368	0.000200
H	-0.828740	-2.057977	0.000076
H	-1.815432	2.132150	-0.000300
H	0.593275	2.759852	-0.000189
H	2.167113	-2.532833	0.000231
N	2.619440	0.728224	0.000094
H	3.177471	1.567562	0.000042
H	4.184288	-0.734335	0.000664
Cl	-3.148884	-0.381724	-0.000213

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -823.413095974 Predicted Change= -1.741906D-07
Zero-point correction (ZPE)= -823.2927 0.12033
Internal Energy (U)= -823.2852 0.12788
Enthalpy (H)= -823.2842 0.12883
Gibbs Free Energy (G)= -823.3253 0.08779

Frequencies -- 122.0614 225.9338 237.8757

Supporting Information: **5radicalindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6N(2) C1[X(C8H6N)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -363.128783467 Predicted Change= -2.688301D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00087	0.00180	[YES]	0.00087	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.232206	0.679250	0.000082
C	0.863773	-0.698783	0.000098
C	-0.511228	-1.035207	-0.000080
C	-1.384236	0.020294	-0.000244
C	-1.059377	1.373098	-0.000269
C	0.294267	1.718927	-0.000091
C	3.116582	-0.559573	0.000059
C	2.082191	-1.458677	0.000499
H	-0.839278	-2.071654	0.000011
H	-1.824153	2.144719	-0.000379
H	0.604304	2.761564	-0.000079
H	2.175896	-2.535829	0.000756
N	2.613346	0.726941	0.000297
H	3.167888	1.568370	0.000378
H	4.184731	-0.727910	-0.000015

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -363.128783467 Predicted Change= -2.688301D-07
Zero-point correction (ZPE)= -363.0119 0.11687
Internal Energy (U)= -363.0055 0.12320
Enthalpy (H)= -363.0046 0.12414
Gibbs Free Energy (G)= -363.0428 0.08592

Frequencies -- 215.5056 256.3762 360.8812

Supporting Information: **6chloroindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6ClN C1[X(C8H6ClN)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -823.413147919 Predicted Change= -1.926833D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00132	0.00180	[YES]	0.00132	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.866762	-0.606459	0.000060
C	-1.269640	0.759352	0.000146
C	-0.275353	1.752350	0.000069
C	1.063006	1.383805	-0.000080
C	1.418109	0.021344	-0.000154
C	0.476197	-0.997614	-0.000090
C	-3.118385	-0.535782	0.000504
C	-2.706076	0.769921	0.000255
H	-0.546686	2.804624	0.000109
H	1.844145	2.136023	-0.000152
H	0.778396	-2.039583	-0.000160
H	-4.116017	-0.952330	0.000727
H	-3.349039	1.639152	0.000295
N	-2.014194	-1.370460	0.000139
H	-2.045468	-2.377945	0.000084
Cl	3.129850	-0.405778	-0.000361

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -823.413147919 Predicted Change= -1.926833D-07
Zero-point correction (ZPE)= -823.2928 0.12034
Internal Energy (U)= -823.2852 0.12788
Enthalpy (H)= -823.2843 0.12883
Gibbs Free Energy (G)= -823.3253 0.08781

Frequencies -- 121.2671 237.1976 239.0679

Supporting Information: **6radicalindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6N(2) C1[X(C8H6N)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -363.128852988 Predicted Change= -7.560630D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 ‖	0.00045	[YES]	0.00001 ‖	0.00030	[YES]
Displ	0.00093 ‖	0.00180	[YES]	0.00093 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.865788	-0.617644	0.000044
C	-1.260976	0.752822	0.000172
C	-0.274355	1.755737	0.000142
C	1.073747	1.392256	-0.000014
C	1.375901	0.034711	-0.000152
C	0.486586	-1.009385	-0.000138
C	-3.119247	-0.533734	0.000658
C	-2.699166	0.768613	0.000096
H	-0.557842	2.805862	0.000168
H	1.852465	2.149748	-0.000099
H	0.791297	-2.053070	-0.000260
H	-4.119359	-0.944537	0.000990
H	-3.337662	1.641323	-0.000002
N	-2.018415	-1.374591	0.000114
H	-2.054954	-2.381713	0.000035

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -363.128852988 Predicted Change= -7.560630D-08
Zero-point correction (ZPE)= -363.0119 0.11687
Internal Energy (U)= -363.0056 0.12318
Enthalpy (H)= -363.0047 0.12413
Gibbs Free Energy (G)= -363.0429 0.08592

Frequencies -- 221.2608 246.8425 375.3729

Supporting Information: **7chloroindole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6ClN C1[X(C8H6ClN)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -823.414237784 Predicted Change= -1.871508D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00122	0.00180	[YES]	0.00122	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.245879	-0.358296	0.000024
C	-1.391038	0.488341	0.000123
C	-1.206971	1.882218	0.000059
C	0.083919	2.393250	-0.000093
C	1.212931	1.547901	-0.000187
C	1.046379	0.172008	-0.000129
C	-2.067641	-1.668621	0.000469
C	-2.535486	-0.380916	0.000217
H	-2.064001	2.550031	0.000107
H	0.239083	3.468339	-0.000155
H	2.214110	1.965545	-0.000313
H	-3.574671	-0.082421	0.000253
N	-0.684920	-1.660236	0.000103
H	-0.083237	-2.469366	0.000041
H	-2.606273	-2.605879	0.000689
Cl	2.428950	-0.921170	-0.000249

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -823.414237784 Predicted Change= -1.871508D-07
Zero-point correction (ZPE)= -823.2937 0.12049
Internal Energy (U)= -823.2862 0.12802
Enthalpy (H)= -823.2852 0.12896
Gibbs Free Energy (G)= -823.3262 0.08799

Frequencies -- 150.5510 199.5415 212.6912

Supporting Information: **7radicalindole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H6N(2) C1[X(C8H6N)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -363.128398140 Predicted Change= -2.263480D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00093	0.00180	[YES]	0.00093	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.238683	-0.369067	0.000110
C	-1.388108	0.484015	0.000134
C	-1.198901	1.879656	-0.000039
C	0.087299	2.401146	-0.000225
C	1.227376	1.553150	-0.000228
C	1.021132	0.198830	-0.000052
C	-2.070279	-1.673749	0.000053
C	-2.533245	-0.384026	0.000542
H	-2.058279	2.545011	0.000047
H	0.235049	3.478205	-0.000301
H	2.226210	1.981317	-0.000308
H	-3.572248	-0.083531	0.000809
N	-0.688401	-1.672421	0.000318
H	-0.097782	-2.488868	0.000396
H	-2.614836	-2.607770	-0.000047

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -363.128398140 Predicted Change= -2.263480D-07
Zero-point correction (ZPE)= -363.0113 0.11704
Internal Energy (U)= -363.0050 0.12335
Enthalpy (H)= -363.0040 0.12430
Gibbs Free Energy (G)= -363.0423 0.08607

Frequencies -- 206.6559 245.2813 371.1939

Chloroisoquinolines

Supporting Information: **1chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17

Charge = 0 Multiplicity = 1

SCF Energy= -861.526885066 Predicted Change= -6.723997D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00108	0.00180	[YES]	0.00108	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.530520	-0.939991	0.000290
C	-3.153295	-0.931833	0.000124
C	-2.445950	0.296770	0.000247
C	-3.177606	1.528225	0.000547
C	-4.596539	1.481933	0.000712
C	-5.257453	0.274689	0.000587
H	-5.065329	-1.885425	0.000191
H	-2.596278	-1.861726	-0.000104
C	-2.447295	2.745446	0.000667
H	-5.150246	2.417253	0.000944
H	-6.343707	0.249568	0.000715
C	-1.021647	0.423790	0.000098
C	-1.075907	2.704620	0.000499
H	-0.481279	3.614385	0.000585
N	-0.363268	1.543758	0.000216
H	-2.973550	3.695595	0.000894
Cl	-0.037891	-1.050149	-0.000261

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.526885066 Predicted Change= -6.723997D-07

Zero-point correction (ZPE)= -861.4004 0.12642

Internal Energy (U)= -861.3925 0.13430

Enthalpy (H)= -861.3916 0.13524

Gibbs Free Energy (G)= -861.4337 0.09314

Frequencies -- 107.4642 176.1705 224.7641

Supporting Information: **1radicalisoquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.252371420 Predicted Change= -1.203084D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00172	0.00180	[YES]	0.00172	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.529881	-0.946998	0.000288
C	-3.151411	-0.934465	0.000123
C	-2.456618	0.297924	0.000252
C	-3.182725	1.535883	0.000551
C	-4.600358	1.483663	0.000714
C	-5.254162	0.269474	0.000585
H	-5.067806	-1.890724	0.000190
H	-2.579247	-1.857489	-0.000105
C	-2.436772	2.751069	0.000670
H	-5.163872	2.413616	0.000943
H	-6.340566	0.242204	0.000711
C	-1.044093	0.434647	0.000105
C	-1.065196	2.715367	0.000497
H	-0.462155	3.618705	0.000580
N	-0.386018	1.520225	0.000211
H	-2.958989	3.703955	0.000898

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.252371420 Predicted Change= -1.203084D-06
Zero-point correction (ZPE)= -401.1290 0.12328
Internal Energy (U)= -401.1224 0.12995
Enthalpy (H)= -401.1214 0.13089
Gibbs Free Energy (G)= -401.1608 0.09150

Frequencies -- 173.2213 189.1379 364.0997

Supporting Information: **3chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.526510235 Predicted Change= -7.290932D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00026	0.00180	[YES]	0.00026	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.518208	-0.943919	0.000284
C	-3.142653	-0.918060	0.000123
C	-2.452879	0.322051	0.000257
C	-3.193308	1.544723	0.000557
C	-4.613261	1.486064	0.000717
C	-5.255352	0.268651	0.000583
H	-5.047907	-1.892181	0.000181
H	-2.568403	-1.841326	-0.000107
C	-2.461635	2.758170	0.000678
H	-5.181052	2.412806	0.000946
H	-6.341299	0.230627	0.000706
C	-1.036919	0.416915	0.000104
H	-0.439787	-0.495143	-0.000129
C	-1.086706	2.689191	0.000500
N	-0.368165	1.553671	0.000221
H	-2.973286	3.714505	0.000905
Cl	-0.152758	4.183791	0.000648

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.526510235 Predicted Change= -7.290932D-08
Zero-point correction (ZPE)= -861.4002 0.12628
Internal Energy (U)= -861.3923 0.13418
Enthalpy (H)= -861.3913 0.13513
Gibbs Free Energy (G)= -861.4335 0.09293

Frequencies -- 95.6052 184.7121 222.4583

Supporting Information: **3radicalisoquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.248172555 Predicted Change= -1.541636D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00040	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00163	0.00180	[YES]	0.00163	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.515681	-0.943269	0.000284
C	-3.141071	-0.915970	0.000124
C	-2.447581	0.324476	0.000256
C	-3.191724	1.550695	0.000557
C	-4.612263	1.486314	0.000716
C	-5.253822	0.269094	0.000582
H	-5.044080	-1.892328	0.000182
H	-2.567298	-1.839626	-0.000106
C	-2.461233	2.773634	0.000682
H	-5.181305	2.412419	0.000945
H	-6.339933	0.230741	0.000705
C	-1.030792	0.402267	0.000098
H	-0.432529	-0.508444	-0.000131
C	-1.095919	2.665043	0.000498
N	-0.388431	1.562516	0.000222
H	-2.977159	3.729181	0.000910

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.248172555 Predicted Change= -1.541636D-06
Zero-point correction (ZPE)= -401.1250 0.12315
Internal Energy (U)= -401.1183 0.12982
Enthalpy (H)= -401.1174 0.13077
Gibbs Free Energy (G)= -401.1567 0.09138

Frequencies -- 177.1483 195.2897 364.0917

Supporting Information: **4chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.523304790 Predicted Change= -1.116558D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00111	0.00180	[YES]	0.00111	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.522296	-0.945991	0.000287
C	-3.146509	-0.911647	0.000126
C	-2.459127	0.328997	0.000257
C	-3.207844	1.548503	0.000557
C	-4.624721	1.484198	0.000718
C	-5.261310	0.262149	0.000584
H	-5.046466	-1.897314	0.000185
H	-2.566876	-1.831461	-0.000103
C	-2.438661	2.745590	0.000669
H	-5.197416	2.404900	0.000946
H	-6.347138	0.223179	0.000709
C	-1.040035	0.408719	0.000099
C	-1.063168	2.697378	0.000494
H	-0.482077	3.615223	0.000581
N	-0.359952	1.534901	0.000209
H	-0.459754	-0.514741	-0.000131
Cl	-3.232527	4.313539	0.001034

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.523304790 Predicted Change= -1.116558D-06
Zero-point correction (ZPE)= -861.3967 0.12656
Internal Energy (U)= -861.3888 0.13445
Enthalpy (H)= -861.3879 0.13540
Gibbs Free Energy (G)= -861.4300 0.09329

Frequencies -- 121.1852 175.4206 211.3516

Supporting Information: **4radicalisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.241016200 Predicted Change= -1.030242D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00027	0.00180	[YES]	0.00027	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.527753	-0.945564	0.000288
C	-3.150876	-0.922930	0.000124
C	-2.456553	0.313293	0.000254
C	-3.206346	1.539886	0.000554
C	-4.625669	1.484172	0.000717
C	-5.266055	0.264953	0.000586
H	-5.057147	-1.894180	0.000187
H	-2.580147	-1.848664	-0.000105
C	-2.426392	2.704176	0.000659
H	-5.188625	2.412514	0.000946
H	-6.351913	0.225380	0.000711
C	-1.035999	0.415398	0.000100
C	-1.066951	2.724060	0.000500
H	-0.477589	3.636265	0.000584
N	-0.361235	1.544644	0.000212
H	-0.444099	-0.500819	-0.000130

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.241016200 Predicted Change= -1.030242D-07
Zero-point correction (ZPE)= -401.1177 0.12321
Internal Energy (U)= -401.1111 0.12987
Enthalpy (H)= -401.1101 0.13081
Gibbs Free Energy (G)= -401.1495 0.09142

Frequencies -- 171.8528 189.0968 356.3176

Supporting Information: **5chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.523324508 Predicted Change= -9.768408D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00086	0.00180	[YES]	0.00086	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.521044	-0.939361	0.000288
C	-3.145547	-0.911395	0.000127
C	-2.460588	0.329094	0.000258
C	-3.188428	1.560364	0.000557
C	-4.609769	1.479508	0.000716
C	-5.261468	0.266732	0.000585
H	-5.054646	-1.885197	0.000188
H	-2.569440	-1.832998	-0.000103
C	-2.433466	2.760800	0.000671
H	-6.346011	0.240577	0.000711
C	-1.039066	0.408517	0.000099
C	-1.059685	2.691977	0.000492
H	-0.463697	3.601634	0.000576
N	-0.350587	1.528879	0.000207
H	-2.936578	3.721034	0.000898
H	-0.465962	-0.520092	-0.000131
Cl	-5.566286	2.955765	0.001088

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.523324508 Predicted Change= -9.768408D-07
Zero-point correction (ZPE)= -861.3967 0.12655
Internal Energy (U)= -861.3888 0.13444
Enthalpy (H)= -861.3879 0.13538
Gibbs Free Energy (G)= -861.4300 0.09328

Frequencies -- 120.7945 175.2577 215.2892

Supporting Information: **5radicalisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.240699530 Predicted Change= -2.819828D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.530632	-0.940828	0.000289
C	-3.153584	-0.911922	0.000128
C	-2.450625	0.322007	0.000255
C	-3.179734	1.559944	0.000555
C	-4.576311	1.440480	0.000703
C	-5.276860	0.275880	0.000588
H	-5.061469	-1.889360	0.000190
H	-2.584250	-1.838030	-0.000102
C	-2.432882	2.766169	0.000672
H	-6.363553	0.252323	0.000715
C	-1.030352	0.409571	0.000097
C	-1.059004	2.699951	0.000494
H	-0.461973	3.609100	0.000578
N	-0.349728	1.536204	0.000208
H	-2.946537	3.722382	0.000900
H	-0.448487	-0.513798	-0.000132

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.240699530 Predicted Change= -2.819828D-07
Zero-point correction (ZPE)= -401.1175 0.12310
Internal Energy (U)= -401.1109 0.12976
Enthalpy (H)= -401.1099 0.13071
Gibbs Free Energy (G)= -401.1493 0.09131

Frequencies -- 170.9064 190.3021 357.4951

Supporting Information: **6chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.524490016 Predicted Change= -8.361025D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00091	0.00180	[YES]	0.00091	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.524290	-0.945191	0.000288
C	-3.149010	-0.914277	0.000127
C	-2.452882	0.321117	0.000255
C	-3.191183	1.542868	0.000554
C	-4.609750	1.496533	0.000718
C	-5.243503	0.275641	0.000585
H	-5.066417	-1.884421	0.000191
H	-2.583488	-1.842827	-0.000103
C	-2.446248	2.751009	0.000671
H	-5.184023	2.417316	0.000946
C	-1.033588	0.406806	0.000097
C	-1.072021	2.694214	0.000494
H	-0.481128	3.607380	0.000579
N	-0.355151	1.535057	0.000208
H	-2.960765	3.708059	0.000900
H	-0.450463	-0.515655	-0.000133
Cl	-6.998756	0.207451	0.000784

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.524490016 Predicted Change= -8.361025D-07
Zero-point correction (ZPE)= -861.3980 0.12639
Internal Energy (U)= -861.3901 0.13430
Enthalpy (H)= -861.3892 0.13525
Gibbs Free Energy (G)= -861.4314 0.09304

Frequencies -- 101.0425 184.8573 218.4319

Supporting Information: **6radicalisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.241566479 Predicted Change= -7.053898D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00038	0.00180	[YES]	0.00038	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.531938	-0.957262	0.000286
C	-3.149457	-0.919644	0.000126
C	-2.462162	0.323552	0.000257
C	-3.193999	1.552937	0.000556
C	-4.622703	1.504734	0.000722
C	-5.196543	0.273246	0.000579
H	-5.070894	-1.900350	0.000188
H	-2.573366	-1.842788	-0.000104
C	-2.443767	2.756418	0.000672
H	-5.199365	2.426534	0.000951
C	-1.042052	0.406980	0.000099
C	-1.069171	2.693611	0.000493
H	-0.474810	3.604798	0.000577
N	-0.357967	1.532110	0.000208
H	-2.953794	3.715964	0.000899
H	-0.461921	-0.517211	-0.000131

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.241566479 Predicted Change= -7.053898D-08
Zero-point correction (ZPE)= -401.1186 0.12295
Internal Energy (U)= -401.1119 0.12962
Enthalpy (H)= -401.1109 0.13056
Gibbs Free Energy (G)= -401.1503 0.09118

Frequencies -- 176.3576 194.2247 363.7631

Supporting Information: **7chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.524186941 Predicted Change= -8.121701D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029 ‖	0.00045	[YES]	0.00006 ‖	0.00030	[YES]
Displ	0.00089 ‖	0.00180	[YES]	0.00089 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.514563	-0.928595	0.000289
C	-3.139931	-0.920540	0.000124
C	-2.454655	0.320692	0.000255
C	-3.190514	1.543582	0.000554
C	-4.609325	1.485322	0.000716
C	-5.262908	0.274445	0.000587
H	-2.579506	-1.850225	-0.000105
C	-2.446029	2.750671	0.000671
H	-5.179854	2.410400	0.000944
H	-6.346517	0.225602	0.000709
C	-1.033528	0.405990	0.000098
C	-1.071570	2.695263	0.000494
H	-0.479470	3.607498	0.000579
N	-0.357186	1.534742	0.000209
H	-2.961368	3.707460	0.000899
H	-0.450151	-0.516075	-0.000132
Cl	-5.384058	-2.456039	0.000130

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.524186941 Predicted Change= -8.121701D-07
Zero-point correction (ZPE)= -861.3977 0.12638
Internal Energy (U)= -861.3898 0.13430
Enthalpy (H)= -861.3889 0.13524
Gibbs Free Energy (G)= -861.4311 0.09303

Frequencies -- 102.9300 183.8936 216.2890

Supporting Information: **7radicalisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.241186074 Predicted Change= -7.857459D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.495360	-0.886550	0.000295
C	-3.138061	-0.936186	0.000121
C	-2.446677	0.313483	0.000252
C	-3.192186	1.534090	0.000552
C	-4.613615	1.488189	0.000716
C	-5.276263	0.273848	0.000588
H	-2.577167	-1.867996	-0.000108
C	-2.449432	2.743275	0.000670
H	-5.174484	2.420291	0.000945
H	-6.361971	0.229833	0.000712
C	-1.026969	0.405822	0.000096
C	-1.074662	2.694660	0.000495
H	-0.487462	3.610182	0.000582
N	-0.355479	1.538169	0.000209
H	-2.967538	3.698739	0.000898
H	-0.439748	-0.513617	-0.000133

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.241186074 Predicted Change= -7.857459D-08
Zero-point correction (ZPE)= -401.1182 0.12296
Internal Energy (U)= -401.1115 0.12963
Enthalpy (H)= -401.1106 0.13057
Gibbs Free Energy (G)= -401.1499 0.09119

Frequencies -- 176.1132 194.7521 362.8604

Supporting Information: **8chloroisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.522432409 Predicted Change= -7.313924D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00121	0.00180	[YES]	0.00121	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.531540	-0.940096	0.000289
C	-3.155733	-0.915435	0.000126
C	-2.433960	0.311034	0.000251
C	-3.184200	1.530119	0.000550
C	-4.602602	1.486020	0.000715
C	-5.255993	0.275658	0.000586
H	-5.054914	-1.889968	0.000188
C	-2.447929	2.743010	0.000670
H	-5.160183	2.418525	0.000944
H	-6.341672	0.238845	0.000711
C	-1.013583	0.412844	0.000097
C	-1.074449	2.703801	0.000496
H	-0.491758	3.622221	0.000583
N	-0.350706	1.551008	0.000211
H	-2.975753	3.692894	0.000898
H	-0.417578	-0.496626	-0.000132
Cl	-2.289439	-2.447157	-0.000243

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.522432409 Predicted Change= -7.313924D-07
Zero-point correction (ZPE)= -861.3959 0.12650
Internal Energy (U)= -861.3880 0.13440
Enthalpy (H)= -861.3870 0.13534
Gibbs Free Energy (G)= -861.4292 0.09322

Frequencies -- 118.8141 175.4623 216.4568

Supporting Information: **8radicalisoquinoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.240834944 Predicted Change= -2.225287D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00049	0.00180	[YES]	0.00049	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.528495	-0.959884	0.000285
C	-3.173009	-0.865154	0.000138
C	-2.432662	0.322450	0.000253
C	-3.187409	1.545427	0.000554
C	-4.607347	1.479327	0.000715
C	-5.259942	0.265606	0.000584
H	-5.050117	-1.913026	0.000183
C	-2.442175	2.752418	0.000671
H	-5.174923	2.406168	0.000943
H	-6.346745	0.231334	0.000710
C	-1.011844	0.411942	0.000096
C	-1.067318	2.701369	0.000495
H	-0.480867	3.617492	0.000581
N	-0.344156	1.546431	0.000209
H	-2.958712	3.708855	0.000899
H	-0.426832	-0.506900	-0.000133

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.240834944 Predicted Change= -2.225287D-07
Zero-point correction (ZPE)= -401.1177 0.12309
Internal Energy (U)= -401.1110 0.12975
Enthalpy (H)= -401.1101 0.13070
Gibbs Free Energy (G)= -401.1495 0.09130

Frequencies -- 171.4010 189.1594 358.4107

Chloroisothiazoles

Supporting Information: **35dichloroisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1488.22382227 Predicted Change= -4.149773D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00109	0.00180	[YES]	0.00109	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.198684	-0.026305	0.000159
C	0.094551	-0.930741	0.000184
C	-1.062785	-0.202817	-0.000023
S	-0.699247	1.495648	0.000344
H	0.168041	-2.009349	0.000199
N	0.964296	1.259814	-0.000242
Cl	2.847459	-0.592852	-0.000166
Cl	-2.677627	-0.806003	-0.000183

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1488.22382227 Predicted Change= -4.149773D-07
Zero-point correction (ZPE)= -1488.1875 0.03632
Internal Energy (U)= -1488.1813 0.04251
Enthalpy (H)= -1488.1803 0.04345
Gibbs Free Energy (G)= -1488.2192 0.00456

Frequencies -- 156.8884 189.2987 275.2450

Supporting Information: **3chloro5radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1027.94041834 Predicted Change= -4.366330D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00091	0.00180	[YES]	0.00091	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.196285	-0.033396	-0.000310
C	0.090322	-0.943631	-0.000052
C	-1.033065	-0.178356	0.000692
S	-0.716011	1.496164	-0.000353
H	0.159114	-2.022587	0.000139
N	0.964749	1.257285	0.000440
Cl	2.849605	-0.582080	-0.000100

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1027.94041834 Predicted Change= -4.366330D-07
Zero-point correction (ZPE)= -1027.9072 0.03320
Internal Energy (U)= -1027.9022 0.03816
Enthalpy (H)= -1027.9013 0.03911
Gibbs Free Energy (G)= -1027.9372 0.00313

Frequencies -- 224.4529 300.9737 427.9788

Supporting Information: **3chloroisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1028.63528034 Predicted Change= -9.207081D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ‖	0.00045	[YES]	0.00003 ‖	0.00030	[YES]
Displ	0.00070 ‖	0.00180	[YES]	0.00070 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.533395	0.028120	-0.000137
C	0.120646	1.298513	0.000044
C	1.473385	1.107517	0.000033
S	1.813375	-0.584866	-0.000053
H	-0.390058	2.252377	0.000076
H	2.255982	1.855667	0.000057
N	0.200011	-1.053874	0.000179
Cl	-2.273166	-0.116351	-0.000011

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1028.63528034 Predicted Change= -9.207081D-08
Zero-point correction (ZPE)= -1028.5895 0.04574
Internal Energy (U)= -1028.5845 0.05072
Enthalpy (H)= -1028.5836 0.05167
Gibbs Free Energy (G)= -1028.6189 0.01629

Frequencies -- 220.9578 302.8590 433.4305

Supporting Information: **3chloroisothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.356792051 Predicted Change= -2.354405D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00086	0.00180	[YES]	0.00086	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.508503	0.020698	0.000031
C	0.114042	1.303447	0.000053
C	1.469937	1.105764	-0.000006
S	1.840287	-0.586274	0.000112
H	-0.392799	2.258736	0.000079
H	2.252334	1.855559	-0.000016
N	0.164649	-1.054477	-0.000053

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.356792051 Predicted Change= -2.354405D-07
Zero-point correction (ZPE)= -568.3145 0.04226
Internal Energy (U)= -568.3105 0.04624
Enthalpy (H)= -568.3096 0.04719
Gibbs Free Energy (G)= -568.3422 0.01449

Frequencies -- 453.8326 534.5989 576.8851

Supporting Information: **4chloroisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1028.63202444 Predicted Change= -5.500706D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00263	0.00180	[NO]	0.00263	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.140985	1.239043	0.000034
C	0.573781	0.002562	0.000018
C	-0.280757	-1.066442	0.000179
S	-1.894945	-0.468474	-0.000094
H	0.328369	2.218447	-0.000014
H	-0.033565	-2.119374	0.000259
N	-1.452436	1.154942	0.000086
Cl	2.310537	-0.102297	-0.000043

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1028.63202444 Predicted Change= -5.500706D-07
Zero-point correction (ZPE)= -1028.5861 0.04584
Internal Energy (U)= -1028.5811 0.05085
Enthalpy (H)= -1028.5802 0.05180
Gibbs Free Energy (G)= -1028.6156 0.01632

Frequencies -- 216.0862 280.0528 429.0315

Supporting Information: **4chloroisothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.346962859 Predicted Change= -5.860697D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00139	0.00180	[YES]	0.00139	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.130999	1.249300	-0.000039
C	0.543769	0.003585	0.000091
C	-0.267503	-1.079850	0.000148
S	-1.895812	-0.469485	-0.000046
H	0.329912	2.231265	0.000007
H	-0.030986	-2.135251	0.000236
N	-1.448918	1.161140	0.000071

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.346962859 Predicted Change= -5.860697D-07
Zero-point correction (ZPE)= -568.3043 0.04261
Internal Energy (U)= -568.3004 0.04649
Enthalpy (H)= -568.2995 0.04743
Gibbs Free Energy (G)= -568.3320 0.01490

Frequencies -- 460.1571 571.7713 619.7942

Supporting Information: **5chloro3radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1027.94653298 Predicted Change= -8.208625D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00152	0.00180	[YES]	0.00152	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.177020	-0.009901	0.000422
C	0.099902	-0.938735	-0.000146
C	-1.057056	-0.202737	0.000364
S	-0.723263	1.510209	-0.000796
H	0.167939	-2.017283	-0.000271
N	0.995091	1.245049	0.000532
Cl	-2.673720	-0.806355	0.000334

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1027.94653298 Predicted Change= -8.208625D-07
Zero-point correction (ZPE)= -1027.9135 0.03294
Internal Energy (U)= -1027.9084 0.03804
Enthalpy (H)= -1027.9075 0.03898
Gibbs Free Energy (G)= -1027.9437 0.00276

Frequencies -- 222.5159 256.1646 428.3774

Supporting Information: **5chloroisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1028.62978717 Predicted Change= -5.334834D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00274	0.00180	[NO]	0.00274	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.693700	1.042986	0.000123
C	0.304470	1.355584	0.000012
C	-0.423397	0.194953	-0.000027
S	0.646544	-1.170050	0.000082
H	2.488537	1.784510	0.000122
H	-0.119150	2.351902	0.000048
N	2.038200	-0.229946	-0.000241
Cl	-2.142949	0.037228	-0.000026

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1028.62978717 Predicted Change= -5.334834D-07
Zero-point correction (ZPE)= -1028.5838 0.04595
Internal Energy (U)= -1028.5788 0.05096
Enthalpy (H)= -1028.5778 0.05191
Gibbs Free Energy (G)= -1028.6133 0.01643

Frequencies -- 221.8902 254.9597 439.0507

Supporting Information: **5chloroisothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.345614008 Predicted Change= -8.216407D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00161	0.00180	[YES]	0.00161	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.690505	1.046126	-0.000297
C	0.297326	1.364330	-0.000066
C	-0.387868	0.186450	0.000479
S	0.628331	-1.179412	-0.000789
H	2.490996	1.782000	-0.000155
H	-0.127879	2.359842	0.000118
N	2.037493	-0.229396	0.000828

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.345614008 Predicted Change= -8.216407D-07
Zero-point correction (ZPE)= -568.3029 0.04268
Internal Energy (U)= -568.2990 0.04656
Enthalpy (H)= -568.2981 0.04751
Gibbs Free Energy (G)= -568.3306 0.01496

Frequencies -- 434.6065 586.3343 610.7474

Chloroisoxazole

Supporting Information: **3chloroisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -705.625326811 Predicted Change= -1.885277D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00099	0.00180	[YES]	0.00099	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.846532	0.591647	0.000019
C	-0.609007	1.150837	0.000027
C	0.240395	0.008186	-0.000033
H	-2.848566	0.996867	-0.000022
H	-0.326345	2.191586	0.000003
N	-0.413497	-1.129232	0.000234
O	-1.758685	-0.752195	-0.000059
Cl	1.966455	0.013512	-0.000073

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.625326811 Predicted Change= -1.885277D-07

Zero-point correction (ZPE)= -705.5766 0.04869

Internal Energy (U)= -705.5720 0.05328

Enthalpy (H)= -705.5710 0.05423

Gibbs Free Energy (G)= -705.6052 0.02008

Frequencies -- 258.8084 313.7286 488.2311

Supporting Information: **3radicalisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -245.339629501 Predicted Change= -2.062271D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00083	0.00180	[YES]	0.00083	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.844037	0.589714	0.000172
C	-0.605889	1.157686	-0.000070
C	0.216127	-0.001653	0.000214
H	-2.843506	1.003756	0.000146
H	-0.326981	2.198850	-0.000164
N	-0.381331	-1.133321	0.000268
O	-1.776621	-0.757336	-0.000398

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -245.339629501 Predicted Change= -2.062271D-07
Zero-point correction (ZPE)= -245.2948 0.04479
Internal Energy (U)= -245.2911 0.04843
Enthalpy (H)= -245.2902 0.04937
Gibbs Free Energy (G)= -245.3216 0.01799

Frequencies -- 574.8769 596.4850 695.8728

Supporting Information: **4chloroisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -705.622973921 Predicted Change= -1.166850D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 ‖	0.00045	[YES]	0.00001 ‖	0.00030	[YES]
Displ	0.00021 ‖	0.00180	[YES]	0.00021 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.564573	-1.086214	0.000008
C	-0.270205	-0.010992	-0.000012
C	0.608347	1.108612	0.000054
H	0.402400	-2.153820	0.000003
N	1.865276	0.736508	-0.000003
H	0.356299	2.161037	0.000069
O	1.839790	-0.663035	0.000080
Cl	-1.997074	0.004298	-0.000058

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.622973921 Predicted Change= -1.166850D-08
Zero-point correction (ZPE)= -705.5741 0.04879
Internal Energy (U)= -705.5695 0.05341
Enthalpy (H)= -705.5686 0.05435
Gibbs Free Energy (G)= -705.6028 0.02009

Frequencies -- 255.9066 290.1389 482.7155

Supporting Information: **4radicalisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -245.333060937 Predicted Change= -7.934613D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00121	0.00180	[YES]	0.00121	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.557931	-1.094039	0.000097
C	-0.253055	-0.010551	0.000070
C	0.598447	1.117372	-0.000132
H	0.403576	-2.162304	0.000029
N	1.859522	0.738078	0.000365
H	0.358980	2.171995	0.000012
O	1.841079	-0.668456	-0.000242

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -245.333060937 Predicted Change= -7.934613D-07
Zero-point correction (ZPE)= -245.2875 0.04550
Internal Energy (U)= -245.2840 0.04905
Enthalpy (H)= -245.2830 0.04999
Gibbs Free Energy (G)= -245.3143 0.01873

Frequencies -- 545.8189 630.2258 818.7626

Supporting Information: **5chloroisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -705.624900368 Predicted Change= -6.566954D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.233558	0.097069	-0.000012
C	0.617847	1.159969	-0.000078
C	1.890486	0.528082	0.000113
H	0.374835	2.210633	-0.000133
N	1.811727	-0.783135	-0.000136
H	2.870458	0.989373	0.000173
O	0.434178	-1.065753	0.000096
Cl	-1.944086	0.005720	0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.624900368 Predicted Change= -6.566954D-08
Zero-point correction (ZPE)= -705.5762 0.04867
Internal Energy (U)= -705.5716 0.05327
Enthalpy (H)= -705.5706 0.05422
Gibbs Free Energy (G)= -705.6048 0.02003

Frequencies -- 235.4618 309.7176 493.1690

Supporting Information: **5radicalisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -245.337436183 Predicted Change= -9.484674D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.208608	0.085049	-0.000074
C	0.615779	1.168726	-0.000023
C	1.888899	0.529018	0.000012
H	0.369382	2.217551	-0.000047
N	1.826282	-0.785455	0.000138
H	2.870093	0.989432	0.000053
O	0.404146	-1.068083	-0.000035

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -245.337436183 Predicted Change= -9.484674D-08
Zero-point correction (ZPE)= -245.2925 0.04492
Internal Energy (U)= -245.2889 0.04853
Enthalpy (H)= -245.2879 0.04947
Gibbs Free Energy (G)= -245.3193 0.01811

Frequencies -- 560.8806 626.3257 694.6866

Chloropyrazoles

Supporting Information: 3chloropyrazole.out

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -685.791977857 Predicted Change= -1.235737D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00169	0.00180	[YES]	0.00169	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.853146	0.650341	0.000047
C	0.571595	1.164890	0.000041
C	-0.249719	0.014971	0.000013
N	1.722541	-0.701450	-0.000012
H	2.453971	-1.396672	-0.000133
H	2.820903	1.131435	0.000107
H	0.265720	2.199483	0.000085
Cl	-1.983184	-0.009995	0.000003
N	0.437945	-1.119341	-0.000090

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.791977857 Predicted Change= -1.235737D-06

Zero-point correction (ZPE)= -685.7300 0.06193

Internal Energy (U)= -685.7252 0.06672

Enthalpy (H)= -685.7243 0.06766

Gibbs Free Energy (G)= -685.7587 0.03324

Frequencies -- 254.6740 317.2280 481.5258

Supporting Information: **4chloropyrazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -685.789776856 Predicted Change= -9.130056D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00102	0.00180	[YES]	0.00102	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.559978	-1.100793	0.000066
C	-0.276469	-0.001289	-0.000017
C	0.573503	1.126459	0.000094
N	1.817484	-0.588829	0.000092
H	2.688945	-1.097518	0.000191
H	0.354266	-2.160625	0.000063
N	1.853602	0.759873	0.000007
H	0.299430	2.172273	0.000110
Cl	-2.010724	-0.015159	-0.000113

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.789776856 Predicted Change= -9.130056D-08
Zero-point correction (ZPE)= -685.7276 0.06209
Internal Energy (U)= -685.7228 0.06690
Enthalpy (H)= -685.7219 0.06784
Gibbs Free Energy (G)= -685.7564 0.03332

Frequencies -- 249.3791 292.2446 480.3857

Supporting Information: **4chloropyrazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -685.789776856 Predicted Change= -9.130056D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00102	0.00180	[YES]	0.00102	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.559978	-1.100793	0.000066
C	-0.276469	-0.001289	-0.000017
C	0.573503	1.126459	0.000094
N	1.817484	-0.588829	0.000092
H	2.688945	-1.097518	0.000191
H	0.354266	-2.160625	0.000063
N	1.853602	0.759873	0.000007
H	0.299430	2.172273	0.000110
Cl	-2.010724	-0.015159	-0.000113

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -685.789776856 Predicted Change= -9.130056D-08
Zero-point correction (ZPE)= -685.7276 0.06209
Internal Energy (U)= -685.7228 0.06690
Enthalpy (H)= -685.7219 0.06784
Gibbs Free Energy (G)= -685.7564 0.03332

Frequencies -- 249.3791 292.2446 480.3857

Supporting Information: **3radicalpyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.503214015 Predicted Change= -7.656590D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00037	0.00180	[YES]	0.00037	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.848625	0.648550	0.000067
C	0.564360	1.170490	0.000031
C	-0.234436	0.007306	0.000032
N	1.727936	-0.706772	-0.000052
H	2.460980	-1.400573	-0.000132
H	2.816390	1.131832	0.000120
H	0.267335	2.207438	0.000072
N	0.424912	-1.114613	-0.000080

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.503214015 Predicted Change= -7.656590D-08
Zero-point correction (ZPE)= -225.4449 0.05828
Internal Energy (U)= -225.4411 0.06208
Enthalpy (H)= -225.4401 0.06303
Gibbs Free Energy (G)= -225.4718 0.03139

Frequencies -- 425.2000 599.9808 651.7509

Supporting Information: **4radicalpyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.498682271 Predicted Change= -4.324446D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00113	0.00180	[YES]	0.00113	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.553898	-1.107843	0.000113
C	-0.261899	-0.000601	0.000062
C	0.562267	1.134155	-0.000082
N	1.816191	-0.594628	0.000019
H	2.693804	-1.093623	-0.000030
H	0.354328	-2.168834	0.000092
N	1.847415	0.757453	0.000471
H	0.304735	2.183471	-0.000039

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.498682271 Predicted Change= -4.324446D-07
Zero-point correction (ZPE)= -225.4399 0.05875
Internal Energy (U)= -225.4361 0.06249
Enthalpy (H)= -225.4352 0.06344
Gibbs Free Energy (G)= -225.4667 0.03191

Frequencies -- 476.6406 564.2682 687.0193

Supporting Information: **5radicalpyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.500111468 Predicted Change= -1.748053D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00089	0.00180	[YES]	0.00089	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.225752	0.088922	-0.000128
C	0.614375	1.179353	0.000049
C	1.894055	0.570884	-0.000129
N	0.501722	-1.039726	-0.000001
H	0.191762	-1.998828	-0.000016
H	0.356297	2.226621	-0.000011
N	1.838964	-0.763655	0.000578
H	2.862313	1.055548	-0.000187

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.500111468 Predicted Change= -1.748053D-07
Zero-point correction (ZPE)= -225.4416 0.05843
Internal Energy (U)= -225.4378 0.06223
Enthalpy (H)= -225.4369 0.06317
Gibbs Free Energy (G)= -225.4685 0.03153

Frequencies -- 408.5610 572.4855 674.8490

Chloropyridazine

Supporting Information: **3chloropyridazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -723.882682499 Predicted Change= -7.051054D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00068	0.00180	[YES]	0.00068	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.461187	-1.262737	-0.000004
C	2.175327	-0.136941	-0.000001
C	1.604469	1.142286	0.000003
C	0.224982	1.220754	0.000003
C	-0.456724	-0.003385	0.000000
N	0.124258	-1.193068	-0.000003
H	2.225512	2.033016	0.000006
H	3.252871	-0.277316	0.000000
H	-0.312684	2.162352	0.000006
Cl	-2.208949	-0.003747	0.000001

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.882682499 Predicted Change= -7.051054D-08

Zero-point correction (ZPE)= -723.8160 0.06658

Internal Energy (U)= -723.8107 0.07190

Enthalpy (H)= -723.8098 0.07284

Gibbs Free Energy (G)= -723.8458 0.03687

Frequencies -- 178.1644 310.5458 383.5197

Supporting Information: **4chloropyridazine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -723.881831939 Predicted Change= -7.726720D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00052	0.00180	[YES]	0.00052	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.563762	-1.214018	-0.000002
C	-0.230386	-1.173927	-0.000003
C	0.490581	0.026011	0.000000
C	-0.223696	1.209443	0.000003
C	-1.617624	1.086111	0.000003
N	-2.267661	-0.080005	0.000000
H	0.276278	-2.134877	-0.000005
H	0.263449	2.178553	0.000005
H	-2.251657	1.969263	0.000005
Cl	2.236390	0.009376	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.881831939 Predicted Change= -7.726720D-08
Zero-point correction (ZPE)= -723.8150 0.06675
Internal Energy (U)= -723.8097 0.07207
Enthalpy (H)= -723.8088 0.07301
Gibbs Free Energy (G)= -723.8448 0.03700

Frequencies -- 181.1366 291.2619 388.9732

Chloropyridines

Supporting Information: **23dichloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-311+g(d,p) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3Cl2N C1[X(C5H3Cl2N)] #Atoms= 11

Charge = 0 Multiplicity = 1

SCF Energy= -1167.59320279 Predicted Change= -1.483940D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00177	0.00180	[YES]	0.00177	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.013279	-0.700281	-0.000011
C	-0.022669	0.702482	0.000048
C	1.188606	1.384901	0.000247
C	2.374905	0.658581	0.000369
C	2.297617	-0.728938	0.000268
N	1.136070	-1.389317	0.000084
H	1.190666	2.467576	0.000306
H	3.334080	1.160841	0.000531
H	3.192402	-1.342324	0.000361
Cl	-1.471226	-1.628050	-0.000308
Cl	-1.515837	1.600912	-0.000122

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1167.59320279 Predicted Change= -1.483940D-06

Zero-point correction (ZPE)= -1167.5239 0.06924

Internal Energy (U)= -1167.5174 0.07577

Enthalpy (H)= -1167.5164 0.07671

Gibbs Free Energy (G)= -1167.5558 0.03736

Frequencies -- 120.3252 202.4454 245.4658

Supporting Information: **24dichloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-311+g(d,p) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3Cl2N C1[X(C5H3Cl2N)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -1167.59777014 Predicted Change= -1.688143D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00147	0.00180	[YES]	0.00147	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.176355	0.024638	-0.000173
C	-0.002619	-0.721820	-0.000069
C	-1.189083	-0.001979	0.000144
C	-1.165059	1.390265	0.000259
C	0.080481	2.006297	0.000172
N	1.241803	1.340126	-0.000048
H	0.011039	-1.801838	-0.000155
H	-2.078061	1.969552	0.000418
H	0.154317	3.088937	0.000244
Cl	2.705328	-0.843535	-0.000391
Cl	-2.715937	-0.851873	0.000262

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1167.59777014 Predicted Change= -1.688143D-06
Zero-point correction (ZPE)= -1167.5285 0.06924
Internal Energy (U)= -1167.5219 0.07577
Enthalpy (H)= -1167.5210 0.07672
Gibbs Free Energy (G)= -1167.5604 0.03728

Frequencies -- 157.6626 200.7835 202.4715

Supporting Information: **25dichloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-311+g(d,p) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3Cl2N C1[X(C5H3Cl2N)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -1167.59635090 Predicted Change= -1.713925D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019 ‖	0.00045	[YES]	0.00004 ‖	0.00030	[YES]
Displ	0.00052 ‖	0.00180	[YES]	0.00052 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.339058	-0.012703	-0.000176
C	-0.699913	1.227990	-0.000116
C	0.688303	1.235583	0.000086
C	1.357547	0.014312	0.000200
C	0.621994	-1.166252	0.000102
N	-0.714249	-1.171792	-0.000082
H	1.239847	2.167297	0.000152
H	-1.269143	2.147512	-0.000220
H	1.117990	-2.130536	0.000193
Cl	-3.096928	-0.059704	-0.000468
Cl	3.106032	-0.044424	0.000457

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1167.59635090 Predicted Change= -1.713925D-07
Zero-point correction (ZPE)= -1167.5271 0.06917
Internal Energy (U)= -1167.5206 0.07574
Enthalpy (H)= -1167.5196 0.07668
Gibbs Free Energy (G)= -1167.5591 0.03720

Frequencies -- 95.3390 221.9742 300.3365

Supporting Information: **2chloro3radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-311+g(d,p) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -707.285322740 Predicted Change= -1.863824D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00014	0.00030	[YES]
Displ	0.00204	0.00180	[NO]	0.00204	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.011314	-0.711325	-0.000238
C	0.021303	0.664171	-0.000013
C	1.181986	1.392598	0.000243
C	2.379096	0.661069	0.000359
C	2.296554	-0.728159	0.000286
N	1.140110	-1.402163	0.000019
H	1.182323	2.477206	0.000349
H	3.341607	1.158844	0.000551
H	3.194666	-1.337102	0.000411
Cl	-1.496859	-1.601598	-0.000138

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.285322740 Predicted Change= -1.863824D-06
Zero-point correction (ZPE)= -707.2194 0.06590
Internal Energy (U)= -707.2140 0.07124
Enthalpy (H)= -707.2131 0.07219
Gibbs Free Energy (G)= -707.2497 0.03556

Frequencies -- 176.9405 298.9632 418.8433

Supporting Information: **2chloro4radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-311+g(d,p) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -707.287808390 Predicted Change= -2.670444D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00049	0.00180	[YES]	0.00049	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.177259	0.019603	-0.000170
C	-0.008928	-0.735829	-0.000060
C	-1.148410	0.021710	0.000148
C	-1.180468	1.395284	0.000264
C	0.077260	2.011021	0.000174
N	1.230256	1.334369	-0.000044
H	0.009308	-1.817578	-0.000144
H	-2.091730	1.980093	0.000429
H	0.156948	3.094320	0.000255
Cl	2.713799	-0.840713	-0.000390

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.287808390 Predicted Change= -2.670444D-07
Zero-point correction (ZPE)= -707.2221 0.06561
Internal Energy (U)= -707.2168 0.07096
Enthalpy (H)= -707.2158 0.07191
Gibbs Free Energy (G)= -707.2525 0.03530

Frequencies -- 171.7581 315.0497 418.4581

Supporting Information: **2chloro5radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-311+g(d,p) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -707.284874929 Predicted Change= -5.156108D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031 ‖	0.00045	[YES]	0.00007 ‖	0.00030	[YES]
Displ	0.00085 ‖	0.00180	[YES]	0.00085 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.330543	-0.011073	-0.000215
C	-0.700785	1.236819	-0.000116
C	0.695596	1.243323	0.000082
C	1.315284	0.014998	0.000195
C	0.636128	-1.179328	0.000150
N	-0.712077	-1.173867	-0.000089
H	1.247488	2.176787	0.000144
H	-1.276987	2.152900	-0.000209
H	1.121707	-2.148053	0.000172
Cl	-3.091738	-0.060729	-0.000450

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.284874929 Predicted Change= -5.156108D-07
Zero-point correction (ZPE)= -707.2190 0.06581
Internal Energy (U)= -707.2137 0.07117
Enthalpy (H)= -707.2127 0.07211
Gibbs Free Energy (G)= -707.2493 0.03550

Frequencies -- 188.4111 310.4813 406.9306

Supporting Information: **2chloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4ClN C1[X(C5H4ClN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -707.883132725 Predicted Change= -8.885343D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00146	0.00180	[YES]	0.00146	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.469882	-0.015670	-0.000041
C	0.197185	1.212709	-0.000003
C	1.589174	1.179347	0.000220
C	2.240415	-0.055755	0.000319
C	1.460420	-1.210271	0.000194
N	0.119421	-1.196715	0.000063
H	2.154605	2.107117	0.000321
H	-0.355543	2.145012	-0.000132
H	3.323520	-0.124222	0.000480
H	1.922041	-2.195485	0.000329
Cl	-2.234379	-0.012799	-0.000328

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.883132725 Predicted Change= -8.885343D-07
Zero-point correction (ZPE)= -707.8037 0.07936
Internal Energy (U)= -707.7984 0.08472
Enthalpy (H)= -707.7974 0.08567
Gibbs Free Energy (G)= -707.8334 0.04964

Frequencies -- 177.5457 312.0599 420.4118

Supporting Information: **3chloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4ClN C1[X(C5H4ClN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -707.879702154 Predicted Change= -4.904332D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00036 ‖	0.00180	[YES]	0.00036 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.208937	-1.191843	-0.000116
C	-0.491022	0.017229	-0.000054
C	0.210337	1.220261	0.000168
C	1.602896	1.158025	0.000313
C	2.219588	-0.093874	0.000205
N	1.543423	-1.249116	0.000012
H	-0.317711	2.168281	0.000223
H	-0.329350	-2.136943	-0.000295
H	2.197920	2.066444	0.000506
H	3.304702	-0.175173	0.000340
Cl	-2.244938	0.009554	-0.000233

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.879702154 Predicted Change= -4.904332D-08
Zero-point correction (ZPE)= -707.8002 0.07944
Internal Energy (U)= -707.7948 0.08481
Enthalpy (H)= -707.7939 0.08576
Gibbs Free Energy (G)= -707.8299 0.04970

Frequencies -- 190.1199 292.1596 414.8015

Supporting Information: **4chloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4ClN C1[X(C5H4ClN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -707.880683575 Predicted Change= -8.240129D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00171	0.00180	[YES]	0.00171	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.593546	-1.140396	0.000004
C	0.199016	-1.204472	-0.000001
C	-0.499760	0.000015	-0.000039
C	0.199028	1.204485	-0.000005
C	1.593559	1.140383	0.000021
N	2.294355	-0.000011	-0.000006
H	2.174603	-2.060773	0.000028
H	-0.318915	-2.157023	0.000008
H	-0.318850	2.157065	-0.000010
H	2.174633	2.060747	0.000004
Cl	-2.252017	-0.000001	0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.880683575 Predicted Change= -8.240129D-07
Zero-point correction (ZPE)= -707.8012 0.07946
Internal Energy (U)= -707.7958 0.08483
Enthalpy (H)= -707.7949 0.08577
Gibbs Free Energy (G)= -707.8309 0.04973

Frequencies -- 188.5891 298.7225 392.8767

Supporting Information: **5chloro2radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-311+g(d,p) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-311+G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -707.291006743 Predicted Change= -7.307429D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00033	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00119	0.00180	[YES]	0.00119	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.315901	-0.016021	-0.000185
C	-0.712592	1.236795	-0.000119
C	0.680450	1.233704	0.000084
C	1.351340	0.007298	0.000198
C	0.632325	-1.181516	0.000110
N	-0.713110	-1.147853	-0.000081
H	1.241942	2.160532	0.000153
H	-1.279179	2.158555	-0.000214
H	1.123584	-2.147083	0.000198
Cl	3.103770	-0.038918	0.000452

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -707.291006743 Predicted Change= -7.307429D-07
Zero-point correction (ZPE)= -707.2249 0.06602
Internal Energy (U)= -707.2196 0.07140
Enthalpy (H)= -707.2186 0.07234
Gibbs Free Energy (G)= -707.2553 0.03569

Frequencies -- 198.6656 294.8749 392.4833

Supporting Information: **pryidine_2_radical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4N(2) C1[X(C5H4N)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -247.606133480 Predicted Change= -1.784211D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00078	0.00180	[YES]	0.00078	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.678370	-0.294436	0.000067
C	-2.286105	-0.353842	-0.000064
C	-1.634786	0.881716	-0.000269
C	-2.390326	2.061959	-0.000413
C	-3.779009	1.972559	-0.000336
N	-4.399781	0.773304	-0.000042
H	-0.547919	0.927430	-0.000336
H	-1.741923	-1.292307	0.000036
H	-1.907015	3.034259	-0.000582
H	-4.411022	2.857428	-0.000374

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -247.606133480 Predicted Change= -1.784211D-07
Zero-point correction (ZPE)= -247.5300 0.07607
Internal Energy (U)= -247.5257 0.08034
Enthalpy (H)= -247.5248 0.08128
Gibbs Free Energy (G)= -247.5580 0.04810

Frequencies -- 387.1699 425.9196 574.5152

Supporting Information: **pryidine_3_radical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4N(2) C1[X(C5H4N)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -247.596916082 Predicted Change= -6.977176D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00044	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00092	0.00180	[YES]	0.00092	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.704393	-0.352771	-0.000050
C	-2.324718	-0.290388	-0.000144
C	-1.615486	0.889656	-0.000373
C	-2.377982	2.066670	-0.000411
C	-3.770176	1.950227	-0.000273
N	-4.426608	0.784378	-0.000116
H	-0.528685	0.919635	-0.000406
H	-4.257723	-1.288422	0.000151
H	-1.903616	3.044854	-0.000528
H	-4.394025	2.842310	-0.000303

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -247.596916082 Predicted Change= -6.977176D-07
Zero-point correction (ZPE)= -247.5209 0.07596
Internal Energy (U)= -247.5167 0.08021
Enthalpy (H)= -247.5157 0.08116
Gibbs Free Energy (G)= -247.5489 0.04798

Frequencies -- 391.3222 423.8404 577.5052

Supporting Information: **pryidine_4_radical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4N(2) C1[X(C5H4N)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -247.598750879 Predicted Change= -1.029398D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00055	0.00180	[YES]	0.00055	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.692658	-0.333318	-0.000022
C	-2.285977	-0.350756	0.000100
C	-1.682815	0.885217	-0.000047
C	-2.374459	2.073933	-0.000254
C	-3.776090	1.954052	-0.000288
N	-4.423157	0.785245	-0.000202
H	-4.244874	-1.272691	0.000072
H	-1.740019	-1.289616	0.000257
H	-1.898517	3.050146	-0.000376
H	-4.395349	2.850652	-0.000480

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -247.598750879 Predicted Change= -1.029398D-07
Zero-point correction (ZPE)= -247.5229 0.07575
Internal Energy (U)= -247.5187 0.08000
Enthalpy (H)= -247.5178 0.08094
Gibbs Free Energy (G)= -247.5509 0.04778

Frequencies -- 379.6164 445.9565 616.3706

Chloropyrimidines

Supporting Information: **24dichloropyrimidine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Cl2N2 C1[X(C4H2Cl2N2)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -1183.51604322 Predicted Change= -3.327912D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00052	0.00180	[YES]	0.00052	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.118308	0.024822	0.000061
N	0.002373	-0.694172	0.000024
C	1.124896	0.006583	0.000009
C	1.158550	1.401818	0.000013
C	-0.085923	2.023735	0.000017
N	-1.242039	1.345077	0.000029
H	2.087600	1.957549	0.000004
H	-0.167264	3.108435	0.000006
Cl	-2.606131	-0.890948	-0.000048
Cl	2.622721	-0.895173	-0.000010

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1183.51604322 Predicted Change= -3.327912D-07

Zero-point correction (ZPE)= -1183.4583 0.05766

Internal Energy (U)= -1183.4520 0.06404

Enthalpy (H)= -1183.4510 0.06498

Gibbs Free Energy (G)= -1183.4902 0.02576

Frequencies -- 162.2527 174.6543 210.3685

Supporting Information: **25dichloropyrimidine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Cl2N2 C1[X(C4H2Cl2N2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -1183.51132781 Predicted Change= -1.970251D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00070	0.00180	[YES]	0.00070	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.307887	0.000001	0.000027
N	-0.724385	1.194343	0.000013
C	0.611304	1.190785	0.000002
C	1.337437	0.000000	-0.000002
C	0.611302	-1.190785	0.000001
N	-0.724385	-1.194343	0.000010
H	1.110381	2.156893	0.000000
H	1.110380	-2.156893	-0.000006
Cl	-3.055200	0.000000	-0.000007
Cl	3.079182	0.000000	-0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1183.51132781 Predicted Change= -1.970251D-07
Zero-point correction (ZPE)= -1183.4536 0.05770
Internal Energy (U)= -1183.4472 0.06412
Enthalpy (H)= -1183.4462 0.06507
Gibbs Free Energy (G)= -1183.4855 0.02577

Frequencies -- 88.7639 222.1060 311.4229

Supporting Information: **2chloro4radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClN2(2) C1[X(C4H2ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -723.240970761 Predicted Change= -2.468860D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00023	0.00180	[YES]	0.00023	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.134078	0.019681	0.000001
N	0.012823	-0.677418	0.000010
C	1.103534	0.013196	0.000016
C	1.172552	1.401398	0.000018
C	-0.080205	2.019563	0.000014
N	-1.236096	1.337268	0.000008
H	2.098567	1.963518	0.000023
H	-0.168351	3.104876	0.000017
Cl	-2.614991	-0.899182	0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.240970761 Predicted Change= -2.468860D-08
Zero-point correction (ZPE)= -723.1864 0.05448
Internal Energy (U)= -723.1812 0.05967
Enthalpy (H)= -723.1803 0.06062
Gibbs Free Energy (G)= -723.2167 0.02423

Frequencies -- 160.9794 329.9945 426.5051

Supporting Information: **2chloro5radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClN2(2) C1[X(C4H2ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -723.227979949 Predicted Change= -3.613127D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00123	0.00180	[YES]	0.00123	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.299254	0.000000	-0.000099
N	-0.724709	1.199258	-0.000025
C	0.622425	1.200014	0.000015
C	1.300009	0.000000	0.000017
C	0.622425	-1.200014	0.000009
N	-0.724709	-1.199257	-0.000028
H	1.111986	2.170378	0.000027
H	1.111985	-2.170378	0.000024
Cl	-3.051212	0.000001	0.000098

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.227979949 Predicted Change= -3.613127D-07
Zero-point correction (ZPE)= -723.1734 0.05448
Internal Energy (U)= -723.1682 0.05970
Enthalpy (H)= -723.1673 0.06064
Gibbs Free Energy (G)= -723.2037 0.02423

Frequencies -- 176.3972 325.4457 403.8496

Supporting Information: **2chloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -723.919929744 Predicted Change= -4.189523D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00028	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00081	0.00180	[YES]	0.00081	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.444394	-0.000001	0.000031
N	-0.133807	-1.196133	0.000012
C	-1.472848	-1.182728	-0.000002
C	-2.209087	0.000000	-0.000006
C	-1.472846	1.182729	-0.000002
N	-0.133806	1.196133	0.000009
H	-1.959361	-2.156189	-0.000003
H	-3.293364	0.000001	-0.000013
H	-1.959359	2.156190	-0.000010
Cl	2.196924	0.000000	-0.000014

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.919929744 Predicted Change= -4.189523D-07
Zero-point correction (ZPE)= -723.8525 0.06742
Internal Energy (U)= -723.8472 0.07266
Enthalpy (H)= -723.8463 0.07360
Gibbs Free Energy (G)= -723.8821 0.03774

Frequencies -- 160.2916 329.6297 414.8915

Supporting Information: **4chloro2radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClN2(2) C1[X(C4H2ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -723.238835336 Predicted Change= -5.138057D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00103	0.00180	[YES]	0.00103	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.091515	0.041278	0.000040
N	-0.006918	-0.699498	0.000031
C	1.126587	-0.001760	0.000017
C	1.148905	1.396442	0.000007
C	-0.090224	2.031749	0.000019
N	-1.247372	1.337573	0.000037
H	2.079244	1.950588	-0.000008
H	-0.165724	3.116966	0.000014
Cl	2.629623	-0.894664	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.238835336 Predicted Change= -5.138057D-07
Zero-point correction (ZPE)= -723.1843 0.05448
Internal Energy (U)= -723.1791 0.05970
Enthalpy (H)= -723.1781 0.06064
Gibbs Free Energy (G)= -723.2146 0.02420

Frequencies -- 171.1117 316.0028 391.4749

Supporting Information: **4chloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -723.921479992 Predicted Change= -2.864851D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00051	0.00180	[YES]	0.00051	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.480500	-1.149822	0.000008
N	-0.140267	-1.186014	0.000002
C	0.464525	-0.011134	0.000008
C	-0.218781	1.205572	0.000004
C	-1.607287	1.108579	0.000005
N	-2.255786	-0.064769	0.000008
H	-1.983451	-2.114078	0.000001
H	0.297826	2.157773	0.000002
H	-2.223847	2.005516	0.000009
Cl	2.219653	-0.012524	-0.000014

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.921479992 Predicted Change= -2.864851D-07
Zero-point correction (ZPE)= -723.8538 0.06762
Internal Energy (U)= -723.8486 0.07286
Enthalpy (H)= -723.8476 0.07381
Gibbs Free Energy (G)= -723.8835 0.03793

Frequencies -- 172.3193 314.1974 384.2936

Supporting Information: **5chloro2radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClN2(2) C1[X(C4H2ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -723.233317228 Predicted Change= -3.717589D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00074	0.00180	[YES]	0.00074	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.278147	0.000001	0.000018
N	-0.734102	1.190957	0.000015
C	0.610040	1.198500	0.000005
C	1.327226	0.000000	-0.000002
C	0.610039	-1.198500	0.000002
N	-0.734103	-1.190957	0.000013
H	1.114800	2.161540	0.000002
H	1.114800	-2.161540	-0.000004
Cl	3.072776	-0.000001	-0.000016

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.233317228 Predicted Change= -3.717589D-07
Zero-point correction (ZPE)= -723.1788 0.05448
Internal Energy (U)= -723.1735 0.05975
Enthalpy (H)= -723.1726 0.06070
Gibbs Free Energy (G)= -723.2091 0.02418

Frequencies -- 200.9630 288.0994 394.6121

Supporting Information: **5chloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -723.916869688 Predicted Change= -7.406350D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00064	0.00180	[YES]	0.00064	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.173564	-0.000001	0.000004
N	1.577300	-1.196708	0.000002
C	0.241170	-1.192972	0.000000
C	-0.480926	0.000000	-0.000002
C	0.241171	1.192973	-0.000004
N	1.577300	1.196709	0.000000
H	-0.265663	-2.155620	0.000002
H	3.261076	0.000001	0.000001
H	-0.265663	2.155620	-0.000002
Cl	-2.227166	0.000000	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.916869688 Predicted Change= -7.406350D-08
Zero-point correction (ZPE)= -723.8492 0.06765
Internal Energy (U)= -723.8439 0.07293
Enthalpy (H)= -723.8429 0.07388
Gibbs Free Energy (G)= -723.8789 0.03794

Frequencies -- 186.2103 286.8821 418.8268

Chloropyrroles

Supporting Information: **23dichloropyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3Cl2N C1[X(C4H3Cl2N)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -1129.35035175 Predicted Change= -2.039637D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00076	0.00180	[YES]	0.00076	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.466816	2.228235	0.000101
C	-0.809433	1.712990	0.000173
C	-0.686247	0.294898	0.000011
C	0.659188	-0.007177	-0.000006
N	1.354007	1.176445	0.000032
H	2.360594	1.243100	-0.000109
H	0.816717	3.249779	0.000140
H	-1.734246	2.271243	0.000280
Cl	1.473510	-1.524391	-0.000103
Cl	-1.985455	-0.850487	-0.000026

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1129.35035175 Predicted Change= -2.039637D-07

Zero-point correction (ZPE)= -1129.2864 0.06393

Internal Energy (U)= -1129.2801 0.07018

Enthalpy (H)= -1129.2792 0.07113

Gibbs Free Energy (G)= -1129.3176 0.03268

Frequencies -- 165.1609 195.1938 240.7339

Supporting Information: **2chloro3radicalypyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN(2) C1[X(C4H3ClN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -669.059113620 Predicted Change= -2.734261D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00138	0.00180	[YES]	0.00138	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.842212	0.652391	0.000140
C	-1.930882	-0.728599	0.000117
C	-0.596531	-1.191510	0.000087
C	0.264366	-0.131437	-0.000013
N	-0.511944	1.009380	-0.000031
H	-0.149752	1.951805	-0.000181
H	-2.616072	1.407002	0.000198
H	-2.839391	-1.313325	0.000188
Cl	1.989434	-0.042130	-0.000116

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -669.059113620 Predicted Change= -2.734261D-07
Zero-point correction (ZPE)= -668.9986 0.06048
Internal Energy (U)= -668.9935 0.06561
Enthalpy (H)= -668.9925 0.06655
Gibbs Free Energy (G)= -669.0282 0.03088

Frequencies -- 196.3571 301.7503 381.4914

Supporting Information: **2chloropyrrole2.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4ClN C1[X(C4H4ClN)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -669.759073228 Predicted Change= -1.160505D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.832165	-0.713209	0.000063
C	1.913868	0.661372	0.000181
C	0.585035	1.180161	-0.000059
C	-0.255281	0.091625	-0.000002
N	0.497273	-1.054999	-0.000002
H	0.119062	-1.989941	-0.000157
H	2.598651	-1.474154	0.000105
H	2.826907	1.240876	0.000316
H	0.279328	2.216282	-0.000120
Cl	-1.985858	0.004249	-0.000072

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -669.759073228 Predicted Change= -1.160505D-07
Zero-point correction (ZPE)= -669.6858 0.07325
Internal Energy (U)= -669.6807 0.07834
Enthalpy (H)= -669.6797 0.07929
Gibbs Free Energy (G)= -669.7147 0.04434

Frequencies -- 216.0730 301.1782 423.1323

Supporting Information: **3chloro2radicalypyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN(2) C1[X(C4H3ClN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -669.057895933 Predicted Change= -3.917482D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00203	0.00180	[NO]	0.00203	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.859817	0.664361	0.000141
C	0.557961	1.112701	-0.000007
C	-0.293661	-0.038115	0.000025
C	0.537871	-1.125342	-0.000106
N	1.836283	-0.720428	-0.000130
H	2.640799	-1.328031	-0.000255
H	2.794869	1.205574	0.000287
H	0.227781	2.142340	0.000025
Cl	-2.028786	-0.038737	0.000031

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -669.057895933 Predicted Change= -3.917482D-07
Zero-point correction (ZPE)= -668.9983 0.05955
Internal Energy (U)= -668.9935 0.06431
Enthalpy (H)= -668.9926 0.06526
Gibbs Free Energy (G)= -669.0276 0.03025

Frequencies -- -124.5800 296.4148 311.4582

Supporting Information: **3chloropyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4ClN C1[X(C4H4ClN)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -669.759876468 Predicted Change= -1.281848D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00074	0.00180	[YES]	0.00074	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.845757	0.713331	0.000062
C	0.543611	1.165227	0.000129
C	-0.282219	0.008336	-0.000015
C	0.521097	-1.110679	-0.000006
N	1.820323	-0.660374	-0.000005
H	2.633879	-1.255822	-0.000155
H	2.779755	1.256031	0.000106
H	0.213751	2.193915	0.000221
H	0.272819	-2.160741	-0.000053
Cl	-2.024232	-0.004003	-0.000065

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -669.759876468 Predicted Change= -1.281848D-07
Zero-point correction (ZPE)= -669.6865 0.07335
Internal Energy (U)= -669.6814 0.07842
Enthalpy (H)= -669.6805 0.07936
Gibbs Free Energy (G)= -669.7154 0.04445

Frequencies -- 238.8488 295.2668 441.3581

Chloroquinazoline

Supporting Information: 2chloroquinazoline.out

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16

Charge = 0 Multiplicity = 1

SCF Energy= -877.566740677 Predicted Change= -1.267219D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.502035	-0.921271	0.000305
C	-3.123819	-0.918716	0.000102
C	-2.426489	0.314842	0.000211
C	-3.167219	1.533322	0.000521
C	-4.583483	1.502377	0.000726
C	-5.238589	0.291098	0.000619
H	-5.038612	-1.866082	0.000224
H	-2.545037	-1.836464	-0.000139
C	-2.391609	2.719975	0.000614
H	-5.137035	2.438168	0.000969
H	-6.324101	0.256952	0.000774
C	-0.494344	1.498625	0.000080
H	-2.881711	3.694194	0.000872
N	-1.060081	0.323248	0.000003
Cl	1.261038	1.527651	0.000054
N	-1.073990	2.722834	0.000427

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.566740677 Predicted Change= -1.267219D-07

Zero-point correction (ZPE)= -877.4524 0.11433

Internal Energy (U)= -877.4446 0.12208

Enthalpy (H)= -877.4437 0.12303

Gibbs Free Energy (G)= -877.4856 0.08104

Frequencies -- 92.5021 174.0292 230.0969

Supporting Information: **2radicalquinazoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.288737051 Predicted Change= -2.401990D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00047	0.00180	[YES]	0.00047	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.504015	-0.923054	0.000305
C	-3.125339	-0.925558	0.000096
C	-2.425139	0.303848	0.000201
C	-3.157552	1.530474	0.000522
C	-4.575290	1.500554	0.000730
C	-5.235198	0.292089	0.000622
H	-5.044282	-1.865885	0.000224
H	-2.550408	-1.845950	-0.000148
C	-2.392206	2.726897	0.000614
H	-5.126679	2.437760	0.000973
H	-6.320874	0.262936	0.000780
C	-0.522376	1.504980	0.000120
H	-2.891990	3.696471	0.000857
N	-1.049027	0.331942	-0.000001
N	-1.067778	2.725598	0.000414

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.288737051 Predicted Change= -2.401990D-07
Zero-point correction (ZPE)= -417.1775 0.11115
Internal Energy (U)= -417.1710 0.11771
Enthalpy (H)= -417.1700 0.11865
Gibbs Free Energy (G)= -417.2093 0.07943

Frequencies -- 169.9891 193.6583 381.9987

Supporting Information: **4chloroquinazoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.568211736 Predicted Change= -3.444833D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00059	0.00180	[YES]	0.00059	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.504863	-0.930099	0.000290
C	-3.127949	-0.910671	0.000107
C	-2.434139	0.325585	0.000231
C	-3.186835	1.542862	0.000538
C	-4.602082	1.495135	0.000724
C	-5.245704	0.277179	0.000602
H	-5.033159	-1.879477	0.000194
H	-2.537645	-1.821067	-0.000131
C	-2.385620	2.721172	0.000618
H	-5.165168	2.421808	0.000960
H	-6.331126	0.239657	0.000739
C	-0.482573	1.494432	0.000260
N	-1.068002	0.321615	0.000051
N	-1.084568	2.718399	0.000475
Cl	-3.170655	4.299429	0.001016
H	0.604783	1.514436	-0.000039

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.568211736 Predicted Change= -3.444833D-07
Zero-point correction (ZPE)= -877.4535 0.11467
Internal Energy (U)= -877.4457 0.12241
Enthalpy (H)= -877.4448 0.12335
Gibbs Free Energy (G)= -877.4867 0.08143

Frequencies -- 104.3000 177.0151 220.6087

Supporting Information: **4radicalquinazoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.294775692 Predicted Change= -2.392063D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.505736	-0.925292	0.000283
C	-3.125964	-0.912387	0.000091
C	-2.429853	0.320775	0.000218
C	-3.191150	1.538995	0.000554
C	-4.603593	1.497523	0.000743
C	-5.249688	0.279090	0.000608
H	-5.033995	-1.874884	0.000173
H	-2.544308	-1.828693	-0.000154
C	-2.385531	2.703374	0.000558
H	-5.157610	2.431452	0.000963
H	-6.335010	0.237601	0.000734
C	-0.466790	1.494953	0.000517
N	-1.061246	0.331719	0.000130
N	-1.113690	2.712054	0.000432
H	0.619513	1.524685	-0.000231

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.294775692 Predicted Change= -2.392063D-07
Zero-point correction (ZPE)= -417.1832 0.11149
Internal Energy (U)= -417.1767 0.11801
Enthalpy (H)= -417.1758 0.11896
Gibbs Free Energy (G)= -417.2149 0.07977

Frequencies -- 174.6322 182.8475 386.3170

Supporting Information: **5chloroquinazoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.563492039 Predicted Change= -2.330198D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00021	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00088	0.00180	[YES]	0.00088	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.504475	-0.919156	0.000290
C	-3.128527	-0.912631	0.000113
C	-2.432952	0.322671	0.000233
C	-3.164003	1.551214	0.000536
C	-4.583693	1.495084	0.000712
C	-5.244864	0.288411	0.000592
H	-5.045466	-1.861178	0.000198
H	-2.545576	-1.827287	-0.000118
C	-2.380780	2.735391	0.000628
C	-0.475744	1.494055	0.000224
H	-2.867194	3.708619	0.000856
N	-1.068311	0.321270	0.000065
N	-1.063678	2.722594	0.000465
H	0.612383	1.496685	-0.000007
H	-6.329215	0.265490	0.000726
Cl	-5.519272	2.983551	0.001081

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.563492039 Predicted Change= -2.330198D-07
Zero-point correction (ZPE)= -877.4487 0.11472
Internal Energy (U)= -877.4409 0.12250
Enthalpy (H)= -877.4400 0.12344
Gibbs Free Energy (G)= -877.4820 0.08146

Frequencies -- 114.2596 180.1157 216.2850

Supporting Information: **5radicalquinazoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.282412304 Predicted Change= -3.298168D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.512385	-0.919438	0.000299
C	-3.134031	-0.911827	0.000120
C	-2.422649	0.316345	0.000228
C	-3.157179	1.551710	0.000524
C	-4.550835	1.457021	0.000691
C	-5.259698	0.296807	0.000592
H	-5.049683	-1.864745	0.000217
H	-2.558858	-1.831702	-0.000108
C	-2.379198	2.739645	0.000650
C	-0.471923	1.501184	0.000049
H	-2.874019	3.710172	0.000888
N	-1.059426	0.324798	0.000025
N	-1.062497	2.729978	0.000453
H	0.616185	1.507276	0.000151
H	-6.345898	0.274008	0.000734

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.282412304 Predicted Change= -3.298168D-07
Zero-point correction (ZPE)= -417.1710 0.11132
Internal Energy (U)= -417.1645 0.11786
Enthalpy (H)= -417.1636 0.11880
Gibbs Free Energy (G)= -417.2028 0.07957

Frequencies -- 170.3441 180.4006 379.6500

Supporting Information: **6chloroquinazoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.564536816 Predicted Change= -1.049108D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00033	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00162	0.00180	[YES]	0.00162	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.505758	-0.927371	0.000294
C	-3.129845	-0.916531	0.000115
C	-2.426225	0.315540	0.000224
C	-3.167151	1.532410	0.000530
C	-4.583806	1.509820	0.000708
C	-5.226621	0.294318	0.000587
H	-5.054099	-1.863441	0.000211
H	-2.556158	-1.837495	-0.000114
C	-2.394881	2.723833	0.000643
H	-5.145120	2.439103	0.000941
C	-0.480405	1.498532	0.000155
H	-2.893656	3.694302	0.000870
N	-1.061774	0.319286	0.000053
N	-1.078800	2.724080	0.000464
Cl	-6.980394	0.230145	0.000807
H	0.607919	1.511797	0.000051

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.564536816 Predicted Change= -1.049108D-06
Zero-point correction (ZPE)= -877.4499 0.11458
Internal Energy (U)= -877.4421 0.12237
Enthalpy (H)= -877.4412 0.12331
Gibbs Free Energy (G)= -877.4832 0.08127

Frequencies -- 103.4398 174.6919 222.2890

Supporting Information: **6radicalquinazoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.281802421 Predicted Change= -8.544767D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00049	0.00180	[YES]	0.00049	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.513731	-0.938752	0.000288
C	-3.130353	-0.921753	0.000111
C	-2.435572	0.317911	0.000233
C	-3.170428	1.542836	0.000536
C	-4.596520	1.519714	0.000720
C	-5.179347	0.292183	0.000585
H	-5.060191	-1.877957	0.000197
H	-2.546137	-1.837162	-0.000120
C	-2.392184	2.729138	0.000626
H	-5.161575	2.449006	0.000947
C	-0.483068	1.495581	0.000234
H	-2.886575	3.701864	0.000855
N	-1.070227	0.319242	0.000067
N	-1.075485	2.723184	0.000466
H	0.605014	1.503149	-0.000013

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.281802421 Predicted Change= -8.544767D-08
Zero-point correction (ZPE)= -417.1706 0.11118
Internal Energy (U)= -417.1640 0.11772
Enthalpy (H)= -417.1631 0.11866
Gibbs Free Energy (G)= -417.2023 0.07945

Frequencies -- 171.7018 191.3399 379.7870

Supporting Information: **7chloroquinazoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.564855860 Predicted Change= -8.091301D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00029	0.00180	[YES]	0.00029	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.498563	-0.909274	0.000292
C	-3.122653	-0.919766	0.000110
C	-2.427618	0.316182	0.000232
C	-3.165312	1.535996	0.000533
C	-4.581923	1.501580	0.000713
C	-5.245271	0.296774	0.000594
H	-2.553342	-1.841835	-0.000121
C	-2.392070	2.724045	0.000623
H	-5.140153	2.434520	0.000940
C	-0.480382	1.497116	0.000243
H	-2.889448	3.695324	0.000851
N	-1.062560	0.317761	0.000068
N	-1.074893	2.724028	0.000467
H	0.607692	1.507323	-0.000018
H	-6.328695	0.251785	0.000725
Cl	-5.378773	-2.426550	0.000145

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.564855860 Predicted Change= -8.091301D-08
Zero-point correction (ZPE)= -877.4502 0.11457
Internal Energy (U)= -877.4424 0.12235
Enthalpy (H)= -877.4415 0.12330
Gibbs Free Energy (G)= -877.4835 0.08126

Frequencies -- 100.4704 182.7572 223.1319

Supporting Information: **7radicalquinazoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.282625678 Predicted Change= -1.804080D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00040	0.00180	[YES]	0.00040	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.476962	-0.864840	0.000311
C	-3.120045	-0.935342	0.000122
C	-2.418216	0.308393	0.000228
C	-3.166926	1.526059	0.000522
C	-4.585884	1.503559	0.000703
C	-5.259052	0.295423	0.000597
H	-2.552756	-1.861072	-0.000105
C	-2.396374	2.716335	0.000650
H	-5.134443	2.443364	0.000937
C	-0.478178	1.501056	-0.000007
H	-2.897864	3.685605	0.000890
N	-1.055187	0.318483	0.000015
N	-1.078884	2.723839	0.000446
H	0.610008	1.516154	0.000201
H	-6.344427	0.254543	0.000740

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.282625678 Predicted Change= -1.804080D-07
Zero-point correction (ZPE)= -417.1714 0.11112
Internal Energy (U)= -417.1649 0.11766
Enthalpy (H)= -417.1640 0.11861
Gibbs Free Energy (G)= -417.2032 0.07941

Frequencies -- 179.8423 182.9018 382.0976

Supporting Information: **8chloroquinazoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.561682217 Predicted Change= -8.172979D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00040 ‖	0.00180	[YES]	0.00040 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.001603	0.007043	-0.000002
C	1.376918	-0.000605	0.000002
C	2.107730	1.223955	0.000005
C	1.363682	2.442402	0.000004
C	-0.052171	2.430870	0.000000
C	-0.719164	1.227520	-0.000003
H	-0.538088	-0.935955	-0.000005
C	2.141105	3.630400	0.000002
H	-0.593577	3.373366	-0.000003
C	4.052095	2.408856	0.000038
H	1.639679	4.599535	-0.000002
N	3.467651	1.231505	0.000014
N	3.456957	3.635168	0.000010
H	5.140037	2.417214	-0.000012
H	-1.804760	1.198608	-0.000007
Cl	2.236147	-1.519786	0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.561682217 Predicted Change= -8.172979D-08
Zero-point correction (ZPE)= -877.4470 0.11465
Internal Energy (U)= -877.4392 0.12242
Enthalpy (H)= -877.4383 0.12336
Gibbs Free Energy (G)= -877.4802 0.08139

Frequencies -- 116.6379 175.9767 204.5584

Supporting Information: **8radicalquinazoline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.278623635 Predicted Change= -2.704237D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00072	0.00180	[YES]	0.00072	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.006221	-0.008928	0.000002
C	1.352312	0.045357	0.000006
C	2.117207	1.223120	0.000007
C	1.366515	2.445939	0.000000
C	-0.052001	2.421841	-0.000005
C	-0.728145	1.222068	-0.000004
H	-0.542685	-0.954540	0.000006
C	2.144741	3.633069	0.000012
H	-0.595083	3.363639	-0.000005
C	4.058881	2.408479	-0.000059
H	1.646214	4.604218	0.000014
N	3.481577	1.227464	-0.000007
N	3.460897	3.634498	0.000003
H	5.146964	2.422277	0.000075
H	-1.814684	1.201381	-0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.278623635 Predicted Change= -2.704237D-07
Zero-point correction (ZPE)= -417.1674 0.11120
Internal Energy (U)= -417.1608 0.11775
Enthalpy (H)= -417.1599 0.11869
Gibbs Free Energy (G)= -417.1991 0.07944

Frequencies -- 171.6890 179.1024 374.2655

Chloroquinolines

Supporting Information: **2chloroquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17

Charge = 0 Multiplicity = 1

SCF Energy= -861.529938911 Predicted Change= -2.627986D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00087	0.00180	[YES]	0.00087	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.495995	-0.922878	0.000309
C	-3.118343	-0.898455	0.000117
C	-2.427855	0.339763	0.000224
C	-3.177206	1.558195	0.000525
C	-4.593948	1.499180	0.000716
C	-5.240013	0.282362	0.000611
H	-5.020840	-1.874210	0.000227
H	-2.527067	-1.808480	-0.000115
C	-2.442509	2.773471	0.000615
H	-5.160411	2.427401	0.000948
H	-6.325626	0.242702	0.000759
C	-1.070135	2.745596	0.000418
C	-0.444660	1.470776	0.000136
H	-2.974468	3.721886	0.000837
H	-0.472169	3.649205	0.000473
N	-1.059605	0.326742	0.000027
Cl	1.323122	1.437621	-0.000165

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.529938911 Predicted Change= -2.627986D-07

Zero-point correction (ZPE)= -861.4037 0.12621

Internal Energy (U)= -861.3958 0.13410

Enthalpy (H)= -861.3948 0.13504

Gibbs Free Energy (G)= -861.4370 0.09290

Frequencies -- 101.2401 176.8232 223.1959

Supporting Information: **2radicalquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.253707761 Predicted Change= -1.155898D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00039 ‖	0.00045	[YES]	0.00008 ‖	0.00030	[YES]
Displ	0.00092 ‖	0.00180	[YES]	0.00092 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.502122	-0.927163	0.000311
C	-3.122878	-0.910138	0.000118
C	-2.433111	0.323648	0.000219
C	-3.168564	1.551242	0.000520
C	-4.585855	1.495634	0.000712
C	-5.238524	0.281422	0.000609
H	-5.032215	-1.875709	0.000233
H	-2.537504	-1.824230	-0.000112
C	-2.435196	2.772744	0.000614
H	-5.149359	2.425789	0.000942
H	-6.324362	0.247843	0.000757
C	-1.057982	2.758345	0.000418
C	-0.459415	1.476002	0.000127
H	-2.979882	3.715416	0.000845
H	-0.468299	3.668541	0.000483
N	-1.055581	0.353866	0.000030

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.253707761 Predicted Change= -1.155898D-06
Zero-point correction (ZPE)= -401.1306 0.12309
Internal Energy (U)= -401.1239 0.12975
Enthalpy (H)= -401.1230 0.13069
Gibbs Free Energy (G)= -401.1623 0.09135

Frequencies -- 173.1186 196.7370 382.5078

Supporting Information: **3chloroquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.525606095 Predicted Change= -4.134085D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00086	0.00180	[YES]	0.00086	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.497075	-0.923486	0.000329
C	-3.120279	-0.897557	0.000134
C	-2.426844	0.340468	0.000208
C	-3.177260	1.559148	0.000500
C	-4.595840	1.500384	0.000703
C	-5.240033	0.283678	0.000615
H	-5.023049	-1.874106	0.000261
H	-2.528606	-1.807440	-0.000087
C	-2.454817	2.779881	0.000591
H	-5.161938	2.428674	0.000932
H	-6.325718	0.244287	0.000767
C	-1.083601	2.727645	0.000390
C	-0.421132	1.471679	0.000088
H	-2.980809	3.729877	0.000812
H	0.667043	1.442330	-0.000068
N	-1.060668	0.323775	0.000015
Cl	-0.120518	4.193608	0.000475

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.525606095 Predicted Change= -4.134085D-07
Zero-point correction (ZPE)= -861.3992 0.12630
Internal Energy (U)= -861.3914 0.13420
Enthalpy (H)= -861.3904 0.13514
Gibbs Free Energy (G)= -861.4326 0.09297

Frequencies -- 98.5368 187.0181 214.8968

Supporting Information: **3radicalquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.242449260 Predicted Change= -5.754867D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00034	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00083	0.00180	[YES]	0.00083	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.495197	-0.922324	0.000326
C	-3.118708	-0.890691	0.000130
C	-2.426688	0.349692	0.000219
C	-3.187074	1.565815	0.000514
C	-4.604160	1.501020	0.000709
C	-5.243384	0.280979	0.000617
H	-5.016560	-1.875567	0.000256
H	-2.524817	-1.799184	-0.000094
C	-2.452476	2.790694	0.000588
H	-5.174672	2.426671	0.000931
H	-6.329095	0.237169	0.000768
C	-1.099131	2.693194	0.000378
C	-0.402872	1.474702	0.000107
H	-2.978763	3.743209	0.000805
H	0.683871	1.427703	-0.000084
N	-1.060899	0.326156	0.000019

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.242449260 Predicted Change= -5.754867D-07
Zero-point correction (ZPE)= -401.1194 0.12299
Internal Energy (U)= -401.1128 0.12964
Enthalpy (H)= -401.1118 0.13058
Gibbs Free Energy (G)= -401.1511 0.09126

Frequencies -- 182.4526 188.4143 381.9929

Supporting Information: **4chloroquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.525672272 Predicted Change= -1.207015D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00172	0.00180	[YES]	0.00172	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.497790	-0.929277	0.000304
C	-3.122491	-0.891925	0.000118
C	-2.430460	0.348080	0.000213
C	-3.192339	1.565371	0.000527
C	-4.609315	1.494677	0.000721
C	-5.245198	0.273515	0.000607
H	-5.016968	-1.883634	0.000220
H	-2.522077	-1.795969	-0.000116
C	-2.438489	2.771775	0.000625
H	-5.183490	2.414756	0.000960
H	-6.330725	0.231129	0.000753
C	-1.065509	2.735730	0.000418
C	-0.430628	1.469518	0.000108
H	-0.479191	3.647487	0.000492
H	0.658114	1.426793	-0.000038
N	-1.065749	0.316980	0.000023
Cl	-3.253670	4.326234	0.000992

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.525672272 Predicted Change= -1.207015D-06
Zero-point correction (ZPE)= -861.3991 0.12648
Internal Energy (U)= -861.3913 0.13433
Enthalpy (H)= -861.3903 0.13527
Gibbs Free Energy (G)= -861.4324 0.09324

Frequencies -- 116.9391 177.2168 217.1971

Supporting Information: **4radicalquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.244482433 Predicted Change= -4.204978D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026 ‖	0.00045	[YES]	0.00005 ‖	0.00030	[YES]
Displ	0.00083 ‖	0.00180	[YES]	0.00083 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.500892	-0.927057	0.000304
C	-3.124157	-0.899252	0.000112
C	-2.425416	0.336575	0.000218
C	-3.194741	1.560028	0.000529
C	-4.612940	1.495881	0.000721
C	-5.250294	0.275598	0.000611
H	-5.022663	-1.880202	0.000220
H	-2.532593	-1.809469	-0.000125
C	-2.424058	2.727457	0.000610
H	-5.178256	2.423034	0.000956
H	-6.335743	0.230368	0.000759
C	-1.068210	2.755561	0.000423
C	-0.425819	1.477211	0.000125
H	-0.478334	3.667421	0.000488
H	0.663832	1.434807	-0.000041
N	-1.062021	0.327046	0.000023

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.244482433 Predicted Change= -4.204978D-07
Zero-point correction (ZPE)= -401.1215 0.12293
Internal Energy (U)= -401.1149 0.12957
Enthalpy (H)= -401.1139 0.13051
Gibbs Free Energy (G)= -401.1532 0.09119

Frequencies -- 174.1872 187.7945 381.4356

Supporting Information: **5chloroquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.525498876 Predicted Change= -1.228251D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00197	0.00180	[NO]	0.00197	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.496059	-0.920199	0.000306
C	-3.121165	-0.892557	0.000131
C	-2.430303	0.347236	0.000221
C	-3.171211	1.576182	0.000517
C	-4.592215	1.492391	0.000704
C	-5.244302	0.281182	0.000595
H	-5.026390	-1.868082	0.000225
H	-2.526404	-1.799840	-0.000089
C	-2.431193	2.786205	0.000604
H	-6.328568	0.251601	0.000730
C	-1.057953	2.733055	0.000407
C	-0.421880	1.466967	0.000114
H	-2.955988	3.735486	0.000823
H	-0.460529	3.639536	0.000471
H	0.666478	1.410559	-0.000027
N	-1.065047	0.317954	0.000038
Cl	-5.553039	2.969704	0.001050

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.525498876 Predicted Change= -1.228251D-06
Zero-point correction (ZPE)= -861.3990 0.12648
Internal Energy (U)= -861.3911 0.13435
Enthalpy (H)= -861.3902 0.13529
Gibbs Free Energy (G)= -861.4322 0.09323

Frequencies -- 116.4217 182.3040 221.7779

Supporting Information: **5radicalquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.243661015 Predicted Change= -3.216854D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00060	0.00180	[YES]	0.00060	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.504033	-0.920683	0.000308
C	-3.127093	-0.893301	0.000126
C	-2.419244	0.339569	0.000223
C	-3.163261	1.575837	0.000515
C	-4.557731	1.454747	0.000684
C	-5.258648	0.290196	0.000598
H	-5.031294	-1.871634	0.000231
H	-2.540489	-1.806161	-0.000096
C	-2.430469	2.790540	0.000605
H	-6.344980	0.262517	0.000740
C	-1.056940	2.739936	0.000410
C	-0.418808	1.473394	0.000131
H	-2.965623	3.735710	0.000823
H	-0.458214	3.645673	0.000467
H	0.669718	1.421647	-0.000030
N	-1.055620	0.319689	0.000036

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.243661015 Predicted Change= -3.216854D-07
Zero-point correction (ZPE)= -401.1206 0.12305
Internal Energy (U)= -401.1139 0.12969
Enthalpy (H)= -401.1130 0.13063
Gibbs Free Energy (G)= -401.1523 0.09129

Frequencies -- 172.9781 185.3567 379.6658

Supporting Information: **7chloroquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.526303519 Predicted Change= -6.256611D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00094	0.00180	[YES]	0.00094	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.491660	-0.907632	0.000309
C	-3.117162	-0.898892	0.000117
C	-2.425967	0.341544	0.000213
C	-3.173543	1.561586	0.000516
C	-4.591603	1.500374	0.000712
C	-5.246614	0.290966	0.000608
H	-2.536967	-1.814249	-0.000111
C	-2.443413	2.776950	0.000614
H	-5.160973	2.426647	0.000948
H	-6.329914	0.240072	0.000753
C	-1.069355	2.734958	0.000415
C	-0.427655	1.470107	0.000114
H	-2.979090	3.723416	0.000845
H	-0.474178	3.642895	0.000487
H	0.661152	1.421858	-0.000032
N	-1.060441	0.314170	0.000026
Cl	-5.356648	-2.437589	0.000187

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.526303519 Predicted Change= -6.256611D-07
Zero-point correction (ZPE)= -861.3999 0.12630
Internal Energy (U)= -861.3921 0.13419
Enthalpy (H)= -861.3911 0.13514
Gibbs Free Energy (G)= -861.4333 0.09298

Frequencies -- 101.5030 187.0534 221.0184

Supporting Information: **7radicalquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.243328641 Predicted Change= -1.732478D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00041	0.00180	[YES]	0.00041	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.471740	-0.864567	0.000312
C	-3.114783	-0.914246	0.000112
C	-2.416065	0.333513	0.000217
C	-3.174855	1.551764	0.000521
C	-4.595289	1.502520	0.000712
C	-5.260473	0.290062	0.000611
H	-2.535650	-1.832817	-0.000119
C	-2.446283	2.768516	0.000616
H	-5.155342	2.435738	0.000943
H	-6.345840	0.244372	0.000756
C	-1.071915	2.733861	0.000417
C	-0.424165	1.473242	0.000126
H	-2.984819	3.713566	0.000845
H	-0.482170	3.645530	0.000480
H	0.664818	1.429449	-0.000039
N	-1.052813	0.314267	0.000024

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.243328641 Predicted Change= -1.732478D-07
Zero-point correction (ZPE)= -401.1204 0.12285
Internal Energy (U)= -401.1138 0.12949
Enthalpy (H)= -401.1128 0.13043
Gibbs Free Energy (G)= -401.1522 0.09112

Frequencies -- 182.9832 186.7028 384.6681

Supporting Information: **8chloroquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6ClN C1[X(C9H6ClN)] #Atoms= 17
Charge = 0 Multiplicity = 1

SCF Energy= -861.523055296 Predicted Change= -2.384586D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.499741	-0.919928	0.000308
C	-3.122508	-0.897195	0.000117
C	-2.403447	0.337038	0.000216
C	-3.167322	1.550726	0.000519
C	-4.584963	1.501577	0.000711
C	-5.234061	0.289141	0.000607
C	-2.442510	2.770813	0.000615
H	-5.145232	2.433068	0.000941
H	-6.319418	0.246393	0.000753
C	-1.069163	2.745381	0.000418
C	-0.417346	1.486807	0.000125
H	-2.988945	3.711069	0.000844
H	-0.484196	3.660079	0.000483
H	0.671467	1.444253	-0.000036
N	-1.043525	0.328236	0.000025
H	-5.018834	-1.872441	0.000226
Cl	-2.241345	-2.407469	-0.000252

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -861.523055296 Predicted Change= -2.384586D-07
Zero-point correction (ZPE)= -861.3966 0.12636
Internal Energy (U)= -861.3888 0.13424
Enthalpy (H)= -861.3878 0.13519
Gibbs Free Energy (G)= -861.4299 0.09311

Frequencies -- 116.8171 177.2821 208.1117

Supporting Information: **8radicalquinoline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H6N(2) C1[X(C9H6N)] #Atoms= 16
Charge = 0 Multiplicity = 2

SCF Energy= -401.239922736 Predicted Change= -1.768086D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00054	0.00180	[YES]	0.00054	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-4.502875	-0.936953	0.000306
C	-3.146932	-0.849310	0.000130
C	-2.395951	0.338940	0.000216
C	-3.165999	1.556945	0.000520
C	-4.585898	1.493009	0.000710
C	-5.242327	0.282495	0.000606
C	-2.439534	2.775685	0.000615
H	-5.149534	2.422822	0.000940
H	-6.328824	0.246913	0.000753
C	-1.065698	2.743970	0.000417
C	-0.411550	1.485290	0.000122
H	-2.981224	3.719169	0.000845
H	-0.478936	3.657679	0.000483
H	0.677628	1.448346	-0.000036
N	-1.031271	0.322732	0.000022
H	-5.020819	-1.892714	0.000223

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -401.239922736 Predicted Change= -1.768086D-07
Zero-point correction (ZPE)= -401.1170 0.12292
Internal Energy (U)= -401.1103 0.12957
Enthalpy (H)= -401.1094 0.13051
Gibbs Free Energy (G)= -401.1487 0.09115

Frequencies -- 174.1662 183.5638 375.5701

Chloroquinoxalines

Supporting Information: **2chloroquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16

Charge = 0 Multiplicity = 1

SCF Energy= -877.563057996 Predicted Change= -9.241329D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00105	0.00180	[YES]	0.00105	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.011736	0.014353	0.000001
C	1.389902	-0.000190	0.000001
C	2.103508	1.222428	0.000001
C	1.386950	2.459322	0.000000
C	-0.029555	2.442763	0.000001
C	-0.701181	1.239611	0.000001
H	-0.538854	-0.922153	0.000001
H	-0.551044	3.394771	0.000001
C	4.058917	2.366208	-0.000002
N	3.471243	1.208596	-0.000001
H	-1.787306	1.224414	0.000001
H	1.957903	-0.924997	0.000000
C	3.360940	3.611324	0.000000
H	3.912189	4.548600	0.000001
N	2.050467	3.654140	0.000000
Cl	5.817996	2.412487	0.000002

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.563057996 Predicted Change= -9.241329D-07

Zero-point correction (ZPE)= -877.4488 0.11417

Internal Energy (U)= -877.4411 0.12192

Enthalpy (H)= -877.4401 0.12287

Gibbs Free Energy (G)= -877.4821 0.08091

Frequencies -- 96.7023 180.8147 222.0606

Supporting Information: **2radicalquinoxaline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.287775116 Predicted Change= -1.458618D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00044	0.00180	[YES]	0.00044	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.005359	0.010456	0.000001
C	1.385265	-0.011381	0.000000
C	2.098061	1.206572	0.000000
C	1.393399	2.452904	0.000000
C	-0.023335	2.439266	0.000001
C	-0.700320	1.238024	0.000001
H	-0.549668	-0.923498	0.000001
H	-0.543253	3.392041	0.000001
C	4.056238	2.368178	-0.000001
N	3.473256	1.240003	0.000000
H	-1.786532	1.228443	0.000001
H	1.946293	-0.940558	0.000000
C	3.374297	3.622750	0.000001
H	3.907548	4.568984	-0.000001
N	2.059206	3.647005	0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.287775116 Predicted Change= -1.458618D-07
Zero-point correction (ZPE)= -417.1766 0.11113
Internal Energy (U)= -417.1701 0.11766
Enthalpy (H)= -417.1691 0.11860
Gibbs Free Energy (G)= -417.2083 0.07946

Frequencies -- 176.2603 192.2354 399.3007

Supporting Information: **3chloroquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.563078948 Predicted Change= -1.000454D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00028	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00157	0.00180	[YES]	0.00157	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.013816	0.014130	0.000001
C	1.391710	0.007138	0.000004
C	2.102588	1.232096	0.000004
C	1.378783	2.464769	0.000000
C	-0.037152	2.444541	-0.000003
C	-0.702291	1.237598	-0.000002
H	-0.533841	-0.923974	0.000001
H	-0.563215	3.393924	-0.000005
C	4.076687	2.383947	0.000006
N	3.469258	1.221949	0.000007
H	5.163679	2.401949	0.000009
H	-1.788461	1.218995	-0.000005
H	1.964523	-0.914811	0.000007
C	3.336093	3.604194	0.000002
N	2.039210	3.662623	0.000000
Cl	4.243440	5.112357	0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.563078948 Predicted Change= -1.000454D-06
Zero-point correction (ZPE)= -877.4489 0.11417
Internal Energy (U)= -877.4411 0.12193
Enthalpy (H)= -877.4402 0.12287
Gibbs Free Energy (G)= -877.4821 0.08091

Frequencies -- 97.1325 180.4152 222.4456

Supporting Information: **3radicalquinoxaline.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.287777888 Predicted Change= -1.480013D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00053	0.00180	[YES]	0.00053	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.012729	0.015769	0.000001
C	1.391597	0.014191	0.000004
C	2.100444	1.240920	0.000004
C	1.361896	2.467480	0.000000
C	-0.049137	2.446119	-0.000003
C	-0.708969	1.233987	-0.000002
H	-0.529947	-0.925222	0.000001
H	-0.582135	3.391644	-0.000006
C	4.093411	2.390032	0.000006
N	3.467597	1.233136	0.000007
H	5.179555	2.388848	0.000009
H	-1.795130	1.210149	-0.000005
H	1.965366	-0.907162	0.000007
C	3.336564	3.600859	0.000003
N	2.067544	3.648319	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.287777888 Predicted Change= -1.480013D-07
Zero-point correction (ZPE)= -417.1766 0.11113
Internal Energy (U)= -417.1701 0.11766
Enthalpy (H)= -417.1691 0.11860
Gibbs Free Energy (G)= -417.2083 0.07946

Frequencies -- 175.8842 192.6801 399.3225

Supporting Information: **5radicalquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.274648555 Predicted Change= -2.313517D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00058	0.00180	[YES]	0.00058	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.006840	0.013306	0.000000
C	1.383721	0.011941	0.000003
C	2.105980	1.234433	0.000004
C	1.394898	2.488455	0.000001
C	-0.005129	2.398084	-0.000002
C	-0.719532	1.241684	-0.000003
H	-0.541301	-0.925432	-0.000001
C	4.079245	2.377582	0.000008
N	3.469676	1.211793	0.000007
H	5.168395	2.372806	0.000010
H	-1.806444	1.234483	-0.000005
H	1.954683	-0.910886	0.000005
C	3.372487	3.611366	0.000006
H	3.921076	4.552279	0.000006
N	2.058750	3.680485	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.274648555 Predicted Change= -2.313517D-07
Zero-point correction (ZPE)= -417.1637 0.11089
Internal Energy (U)= -417.1572 0.11741
Enthalpy (H)= -417.1562 0.11835
Gibbs Free Energy (G)= -417.1954 0.07919

Frequencies -- 172.1073 180.7919 395.2846

Supporting Information: **5chloroquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.556970366 Predicted Change= -2.201497D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00048	0.00180	[YES]	0.00048	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.015132	0.018171	0.000000
C	1.390711	0.007780	0.000003
C	2.101348	1.233738	0.000004
C	1.391948	2.479710	0.000002
C	-0.033552	2.441276	-0.000002
C	-0.703902	1.237972	-0.000003
H	-0.539250	-0.915780	-0.000001
C	4.077057	2.373889	0.000007
N	3.465875	1.209210	0.000007
H	5.166034	2.368017	0.000011
H	-1.788591	1.230546	-0.000005
H	1.963433	-0.913742	0.000005
C	3.369273	3.605766	0.000005
H	3.912420	4.549637	0.000007
N	2.055408	3.666187	0.000002
Cl	-0.936798	3.937767	-0.000006

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.556970366 Predicted Change= -2.201497D-07
Zero-point correction (ZPE)= -877.4426 0.11433
Internal Energy (U)= -877.4348 0.12208
Enthalpy (H)= -877.4339 0.12303
Gibbs Free Energy (G)= -877.4758 0.08112

Frequencies -- 113.9398 183.6064 209.4737

Supporting Information: **6chloroquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.559866040 Predicted Change= -2.515398D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00058	0.00180	[YES]	0.00058	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.012690	0.007778	0.000000
C	1.388020	0.005307	0.000003
C	2.107969	1.227406	0.000005
C	1.386767	2.462299	0.000002
C	-0.031160	2.449472	-0.000002
C	-0.687386	1.241088	-0.000003
H	-0.547815	-0.920857	-0.000001
H	-0.562585	3.394313	-0.000004
C	4.071380	2.377253	0.000007
N	3.471303	1.205423	0.000007
H	5.160277	2.381873	0.000011
H	1.953132	-0.921337	0.000005
C	3.354167	3.604978	0.000005
H	3.894525	4.550615	0.000007
N	2.039249	3.661171	0.000002
Cl	-2.442509	1.201789	-0.000007

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.559866040 Predicted Change= -2.515398D-07
Zero-point correction (ZPE)= -877.4456 0.11426
Internal Energy (U)= -877.4378 0.12202
Enthalpy (H)= -877.4369 0.12296
Gibbs Free Energy (G)= -877.4788 0.08101

Frequencies -- 102.8009 180.0518 226.4523

Supporting Information: **6radicalquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.277145490 Predicted Change= -1.330551D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00041	0.00180	[YES]	0.00041	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.004279	-0.003806	0.000000
C	1.386911	0.000792	0.000003
C	2.098069	1.230847	0.000004
C	1.383812	2.474265	0.000001
C	-0.043728	2.459534	-0.000002
C	-0.639579	1.238787	-0.000003
H	-0.554039	-0.935680	-0.000001
H	-0.579182	3.404341	-0.000004
C	4.068370	2.374998	0.000009
N	3.462329	1.206581	0.000007
H	5.157484	2.374080	0.000010
H	1.962584	-0.920412	0.000005
C	3.358060	3.605715	0.000006
H	3.902315	4.549291	0.000006
N	2.042848	3.667450	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.277145490 Predicted Change= -1.330551D-07
Zero-point correction (ZPE)= -417.1663 0.11082
Internal Energy (U)= -417.1598 0.11733
Enthalpy (H)= -417.1588 0.11828
Gibbs Free Energy (G)= -417.1979 0.07915

Frequencies -- 176.3480 191.0033 400.1170

Supporting Information: **7chloroquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.559864299 Predicted Change= -2.350302D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00051	0.00180	[YES]	0.00051	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.022687	0.024187	-0.000001
C	1.397538	-0.000017	0.000003
C	2.107167	1.227409	0.000005
C	1.387934	2.463438	0.000002
C	-0.030415	2.438954	-0.000002
C	-0.705781	1.240891	-0.000003
H	-0.558537	3.387217	-0.000004
C	4.070830	2.376688	0.000007
N	3.471863	1.204684	0.000007
H	5.159867	2.380372	0.000011
H	-1.789913	1.210607	-0.000005
H	1.958067	-0.927762	0.000005
C	3.355702	3.605620	0.000005
H	3.896753	4.550699	0.000007
N	2.040403	3.660757	0.000002
Cl	-0.876182	-1.483994	-0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.559864299 Predicted Change= -2.350302D-07
Zero-point correction (ZPE)= -877.4456 0.11426
Internal Energy (U)= -877.4378 0.12202
Enthalpy (H)= -877.4369 0.12296
Gibbs Free Energy (G)= -877.4788 0.08100

Frequencies -- 102.7352 179.5773 226.0400

Supporting Information: **7radicalquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.277149641 Predicted Change= -1.354701D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00037	0.00180	[YES]	0.00037	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.044178	0.066916	0.000000
C	1.400041	-0.015995	0.000003
C	2.116205	1.219003	0.000004
C	1.385973	2.453108	0.000001
C	-0.034795	2.440281	-0.000002
C	-0.720002	1.239361	-0.000003
H	-0.552857	3.395068	-0.000004
C	4.073464	2.379531	0.000009
N	3.479211	1.204602	0.000007
H	5.162718	2.388295	0.000010
H	-1.805994	1.212573	-0.000006
H	1.958453	-0.947414	0.000005
C	3.352390	3.603976	0.000006
H	3.888151	4.552200	0.000006
N	2.037029	3.652240	0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.277149641 Predicted Change= -1.354701D-07
Zero-point correction (ZPE)= -417.1663 0.11082
Internal Energy (U)= -417.1598 0.11733
Enthalpy (H)= -417.1588 0.11828
Gibbs Free Energy (G)= -417.1979 0.07916

Frequencies -- 176.1404 191.6287 400.1999

Supporting Information: **8chloroquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5ClN2 C1[X(C8H5ClN2)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -877.556950260 Predicted Change= -1.741260D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014 ‖	0.00045	[YES]	0.00003 ‖	0.00030	[YES]
Displ	0.00052 ‖	0.00180	[YES]	0.00052 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.008932	0.012444	0.000000
C	1.386280	0.001333	0.000003
C	2.123601	1.221784	0.000005
C	1.390064	2.453731	0.000002
C	-0.026992	2.441025	-0.000002
C	-0.697118	1.239722	-0.000003
H	-0.532943	-0.927225	-0.000001
H	-0.545770	3.394000	-0.000004
C	4.078702	2.386083	0.000007
N	3.482993	1.213373	0.000007
H	5.167598	2.392441	0.000010
H	-1.782977	1.218565	-0.000005
C	3.356506	3.609572	0.000005
H	3.889123	4.559503	0.000007
N	2.041986	3.652795	0.000002
Cl	2.240824	-1.523611	0.000006

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -877.556950260 Predicted Change= -1.741260D-07
Zero-point correction (ZPE)= -877.4426 0.11433
Internal Energy (U)= -877.4348 0.12208
Enthalpy (H)= -877.4339 0.12302
Gibbs Free Energy (G)= -877.4758 0.08111

Frequencies -- 114.2676 183.7022 209.2138

Supporting Information: **8radicalquinoxaline.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq nosymm ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H5N2(2) C1[X(C8H5N2)] #Atoms= 15
Charge = 0 Multiplicity = 2

SCF Energy= -417.274651584 Predicted Change= -2.334779D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00055	0.00180	[YES]	0.00055	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.004465	-0.003114	0.000000
C	1.362815	0.047284	0.000003
C	2.132494	1.220261	0.000004
C	1.392799	2.457621	0.000001
C	-0.026866	2.433002	-0.000002
C	-0.705361	1.234892	-0.000003
H	-0.538281	-0.944842	-0.000001
H	-0.547618	3.385060	-0.000004
C	4.085187	2.385954	0.000008
N	3.496851	1.209284	0.000007
H	5.174273	2.398670	0.000010
H	-1.792327	1.221506	-0.000005
C	3.360978	3.609575	0.000006
H	3.894355	4.559196	0.000006
N	2.046221	3.654796	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -417.274651584 Predicted Change= -2.334779D-07
Zero-point correction (ZPE)= -417.1637 0.11090
Internal Energy (U)= -417.1572 0.11741
Enthalpy (H)= -417.1562 0.11836
Gibbs Free Energy (G)= -417.1954 0.07919

Frequencies -- 171.8303 180.9243 395.3959

Chlorooxazoles

Supporting Information: **2chlorooxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -705.659551766 Predicted Change= -1.755875D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00085	0.00180	[YES]	0.00085	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.781309	-0.682708	0.000129
C	1.813516	0.671307	0.000114
C	-0.215390	0.101833	-0.000077
H	2.511624	-1.475422	0.000209
H	2.666275	1.334577	0.000188
N	0.511495	1.168277	0.000015
O	0.459971	-1.070651	0.000049
Cl	-1.924397	-0.000852	-0.000111

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.659551766 Predicted Change= -1.755875D-07

Zero-point correction (ZPE)= -705.6103 0.04919

Internal Energy (U)= -705.6058 0.05375

Enthalpy (H)= -705.6048 0.05469

Gibbs Free Energy (G)= -705.6389 0.02062

Frequencies -- 235.6877 330.4826 506.9654

Supporting Information: **4chlorooxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -705.661278114 Predicted Change= -1.092745D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00041	0.00045	[YES]	0.00015	0.00030	[YES]
Displ	0.00147	0.00180	[YES]	0.00147	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.559319	1.102103	-0.000037
C	0.249676	0.010902	-0.000018
C	-1.724577	-0.711122	0.000072
H	-0.408639	2.168531	-0.000091
H	-2.639142	-1.285635	0.000165
N	-0.503742	-1.145457	0.000104
O	-1.848806	0.639155	0.000054
Cl	1.974691	-0.022896	-0.000079

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.661278114 Predicted Change= -1.092745D-06
Zero-point correction (ZPE)= -705.6119 0.04932
Internal Energy (U)= -705.6073 0.05388
Enthalpy (H)= -705.6064 0.05483
Gibbs Free Energy (G)= -705.6405 0.02073

Frequencies -- 255.8144 317.1647 488.6540

Supporting Information: **5chlorooxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -705.659208744 Predicted Change= -9.468980D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00014	0.00030	[YES]
Displ	0.00147	0.00180	[YES]	0.00147	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.241415	0.099157	-0.000023
C	0.625445	1.144259	0.000007
C	1.770199	-0.642525	0.000114
H	0.411982	2.202422	-0.000034
H	2.525176	-1.414820	0.000208
N	1.921332	0.642052	0.000102
O	0.473791	-1.063679	0.000061
Cl	-1.947187	-0.022229	-0.000116

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.659208744 Predicted Change= -9.468980D-07
Zero-point correction (ZPE)= -705.6098 0.04932
Internal Energy (U)= -705.6053 0.05390
Enthalpy (H)= -705.6043 0.05484
Gibbs Free Energy (G)= -705.6385 0.02070

Frequencies -- 232.0294 309.9802 495.3904

Supporting Information: **2radicaloxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -245.371296762 Predicted Change= -1.214508D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00056	0.00180	[YES]	0.00056	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.783442	-0.683325	0.000120
C	1.816613	0.670901	0.000136
C	-0.197472	0.103803	-0.000053
H	2.513459	-1.476759	0.000188
H	2.667273	1.336925	0.000208
N	0.498441	1.166846	-0.000039
O	0.447043	-1.071178	0.000066

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -245.371296762 Predicted Change= -1.214508D-07
Zero-point correction (ZPE)= -245.3257 0.04559
Internal Energy (U)= -245.3221 0.04916
Enthalpy (H)= -245.3211 0.05010
Gibbs Free Energy (G)= -245.3524 0.01883

Frequencies -- 549.8468 607.9399 744.0515

Supporting Information: **4adicaloxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -245.372737084 Predicted Change= -3.200965D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00118	0.00180	[YES]	0.00118	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.548403	1.104279	0.000128
C	0.234159	0.001297	0.000006
C	-1.726034	-0.710303	0.000423
H	-0.407868	2.171106	0.000099
H	-2.638152	-1.288996	0.000383
N	-0.495567	-1.136359	-0.000200
O	-1.852685	0.637453	-0.000589

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -245.372737084 Predicted Change= -3.200965D-07
Zero-point correction (ZPE)= -245.3267 0.04602
Internal Energy (U)= -245.3231 0.04955
Enthalpy (H)= -245.3222 0.05049
Gibbs Free Energy (G)= -245.3534 0.01930

Frequencies -- 595.3951 657.5187 722.8413

Supporting Information: **5adicaloxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -245.368246790 Predicted Change= -3.220023D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.222705	0.092943	-0.000027
C	0.618407	1.155512	-0.000009
C	1.769176	-0.649146	0.000096
H	0.409284	2.212967	-0.000055
H	2.528685	-1.416816	0.000176
N	1.916395	0.638252	0.000162
O	0.467269	-1.066845	0.000092

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -245.368246790 Predicted Change= -3.220023D-07
Zero-point correction (ZPE)= -245.3224 0.04578
Internal Energy (U)= -245.3189 0.04932
Enthalpy (H)= -245.3179 0.05027
Gibbs Free Energy (G)= -245.3492 0.01904

Frequencies -- 528.4272 663.4536 790.9975

Chlorothiazoles

Supporting Information: **24dichlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -1488.22978446 Predicted Change= -2.616958D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00154	0.00180	[YES]	0.00154	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.899072	1.322739	0.000243
C	1.182142	-0.011710	0.000571
C	-0.983299	-0.207108	0.000851
H	1.583068	2.158749	-0.000111
N	0.121327	-0.879565	0.000401
S	-0.825075	1.537218	-0.000394
Cl	-2.547007	-0.940468	-0.000674
Cl	2.792969	-0.660756	0.000298

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1488.22978446 Predicted Change= -2.616958D-07

Zero-point correction (ZPE)= -1488.1935 0.03627

Internal Energy (U)= -1488.1873 0.04246

Enthalpy (H)= -1488.1863 0.04341

Gibbs Free Energy (G)= -1488.2252 0.00454

Frequencies -- 169.7593 197.6051 243.7779

Supporting Information: **25dichlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1488.22573899 Predicted Change= -1.103799D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00107	0.00180	[YES]	0.00107	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.215729	0.183970	0.000207
C	-0.633985	1.417870	0.000111
C	1.201665	0.215968	0.000661
H	-1.172662	2.357370	-0.000226
N	0.743329	1.422266	-0.000069
S	0.005684	-1.069939	0.000121
Cl	2.886985	-0.173369	-0.000237
Cl	-2.900708	-0.185517	-0.000180

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1488.22573899 Predicted Change= -1.103799D-07
Zero-point correction (ZPE)= -1488.1892 0.03648
Internal Energy (U)= -1488.1829 0.04274
Enthalpy (H)= -1488.1820 0.04368
Gibbs Free Energy (G)= -1488.2210 0.00470

Frequencies -- 115.0769 194.3316 300.1956

Supporting Information: **2chloro4radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1027.94763691 Predicted Change= -9.103943D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00100	0.00180	[YES]	0.00100	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.066380	0.025188	0.000446
C	1.512790	1.257855	0.000041
C	-0.373279	0.229367	-0.000491
H	3.097523	-0.295213	0.000886
N	0.182462	1.406939	-0.000244
S	0.735140	-1.128822	-0.000170
Cl	-2.080726	-0.033334	0.000210

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1027.94763691 Predicted Change= -9.103943D-08
Zero-point correction (ZPE)= -1027.9145 0.03311
Internal Energy (U)= -1027.9095 0.03812
Enthalpy (H)= -1027.9085 0.03906
Gibbs Free Energy (G)= -1027.9446 0.00301

Frequencies -- 219.7998 274.8980 447.5167

Supporting Information: **2chloro5radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1027.94110291 Predicted Change= -1.248741D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00058	0.00180	[YES]	0.00058	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.016843	-0.172292	-0.000108
C	1.672994	1.136249	0.000049
C	-0.338175	0.207898	-0.000083
H	2.334968	1.991821	0.000204
N	0.296350	1.334469	0.000140
S	0.659576	-1.244301	-0.000145
Cl	-2.063095	0.090858	0.000116

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1027.94110291 Predicted Change= -1.248741D-07
Zero-point correction (ZPE)= -1027.9077 0.03332
Internal Energy (U)= -1027.9027 0.03834
Enthalpy (H)= -1027.9018 0.03928
Gibbs Free Energy (G)= -1027.9379 0.00318

Frequencies -- 221.0159 271.8591 445.6717

Supporting Information: **2chlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1028.63821212 Predicted Change= -4.216898D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00168	0.00180	[YES]	0.00168	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.003385	-0.133916	-0.000119
C	-1.578557	1.161752	0.000575
C	0.394865	0.217482	0.000033
H	-3.015037	-0.515629	-0.000195
H	-2.227498	2.029695	0.000831
N	-0.212990	1.356642	-0.000698
S	-0.634120	-1.203926	-0.000031
Cl	2.117756	0.045903	0.000107

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1028.63821212 Predicted Change= -4.216898D-07
Zero-point correction (ZPE)= -1028.5923 0.04590
Internal Energy (U)= -1028.5872 0.05092
Enthalpy (H)= -1028.5863 0.05186
Gibbs Free Energy (G)= -1028.6217 0.01641

Frequencies -- 220.3698 274.8625 446.6289

Supporting Information: **4chloro2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1027.95234815 Predicted Change= -3.959396D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00023	0.00180	[YES]	0.00023	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.337604	-1.012113	0.000121
C	-0.538511	0.032124	0.000127
C	1.288462	1.215210	0.000082
H	0.122483	-2.071109	0.000079
N	0.030090	1.295720	-0.000028
S	1.977069	-0.387595	-0.000069
Cl	-2.264209	-0.129926	-0.000044

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1027.95234815 Predicted Change= -3.959396D-08
Zero-point correction (ZPE)= -1027.9191 0.03317
Internal Energy (U)= -1027.9141 0.03821
Enthalpy (H)= -1027.9131 0.03916
Gibbs Free Energy (G)= -1027.9493 0.00303

Frequencies -- 208.0239 300.0381 431.8788

Supporting Information: **4chlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1028.63971176 Predicted Change= -1.818143D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00123	0.00180	[YES]	0.00123	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.278830	-1.052099	-0.000057
C	-0.559512	0.026133	0.000084
C	1.313131	1.148237	0.000140
H	0.028061	-2.102285	-0.000141
N	0.017494	1.266539	-0.000078
S	1.917003	-0.490270	0.000018
H	1.993991	1.991107	0.000209
Cl	-2.294779	-0.096700	-0.000047

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1028.63971176 Predicted Change= -1.818143D-07
Zero-point correction (ZPE)= -1028.5938 0.04585
Internal Energy (U)= -1028.5888 0.05085
Enthalpy (H)= -1028.5879 0.05179
Gibbs Free Energy (G)= -1028.6233 0.01636

Frequencies -- 209.4030 300.6549 436.1574

Supporting Information: **5chloro2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1027.94988919 Predicted Change= -7.312812D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00169	0.00180	[YES]	0.00169	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.368060	0.190951	-0.000008
C	-0.359952	1.343821	0.000864
C	-2.034790	-0.093466	-0.000903
H	0.039483	2.349671	0.001249
N	-1.733869	1.127854	-0.000362
S	-0.699368	-1.219448	0.000378
Cl	2.085152	0.036394	-0.000264

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1027.94988919 Predicted Change= -7.312812D-07
Zero-point correction (ZPE)= -1027.9165 0.03335
Internal Energy (U)= -1027.9114 0.03844
Enthalpy (H)= -1027.9105 0.03938
Gibbs Free Energy (G)= -1027.9467 0.00315

Frequencies -- 226.6147 254.4622 432.6655

Supporting Information: **5chlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1028.63473024 Predicted Change= -3.732534D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00093	0.00180	[YES]	0.00093	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.415043	0.184300	0.000041
C	-0.310384	1.342023	0.000243
C	-1.992840	-0.081807	-0.000010
H	0.117174	2.337449	0.000262
N	-1.675161	1.178721	-0.000547
S	-0.646130	-1.199916	0.000021
H	-3.011700	-0.452126	-0.000021
Cl	2.134577	0.023247	0.000094

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1028.63473024 Predicted Change= -3.732534D-07
Zero-point correction (ZPE)= -1028.5886 0.04604
Internal Energy (U)= -1028.5836 0.05107
Enthalpy (H)= -1028.5827 0.05201
Gibbs Free Energy (G)= -1028.6182 0.01648

Frequencies -- 220.3342 258.0032 437.1581

Chlorothiophenes

Supporting Information: **23dichlorothiophene_b3lyp.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Cl2S C1[X(C4H2Cl2S)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -1472.18319699 Predicted Change= -7.307955D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00114	0.00180	[YES]	0.00114	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.719404	-1.470785	0.000265
C	0.401623	-1.820816	-0.000070
C	-0.464033	-0.682686	-0.000049
C	0.214910	0.507576	0.000133
S	1.940205	0.252678	-0.000499
H	2.582938	-2.121980	0.000497
H	0.035894	-2.840424	-0.000058
Cl	-0.445470	2.098550	0.000351
Cl	-2.195326	-0.820913	-0.000006

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1472.18319699 Predicted Change= -7.307955D-08

Zero-point correction (ZPE)= -1472.1350 0.04815

Internal Energy (U)= -1472.1286 0.05457

Enthalpy (H)= -1472.1276 0.05551

Gibbs Free Energy (G)= -1472.1668 0.01630

Frequencies -- 158.6518 173.3928 239.1483

Supporting Information: **24dichlorothiophene_b3lyp.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Cl2S C1[X(C4H2Cl2S)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1472.18466886 Predicted Change= -7.559630D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00122	0.00180	[YES]	0.00122	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.916765	1.297391	0.000534
C	1.239242	-0.028397	-0.000017
C	0.115810	-0.912051	-0.000284
C	-1.055272	-0.211141	0.000059
S	-0.807329	1.515222	-0.000276
H	1.582576	2.148501	0.000951
H	0.186398	-1.991904	-0.000487
Cl	-2.655287	-0.868492	0.000144
Cl	2.881700	-0.618270	-0.000015

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1472.18466886 Predicted Change= -7.559630D-08
Zero-point correction (ZPE)= -1472.1366 0.04805
Internal Energy (U)= -1472.1301 0.05448
Enthalpy (H)= -1472.1292 0.05542
Gibbs Free Energy (G)= -1472.1685 0.01613

Frequencies -- 158.9159 187.3045 244.5318

Supporting Information: **2chloro3radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1011.89818345 Predicted Change= -6.040665D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.716205	-1.476195	0.000120
C	0.392931	-1.831557	0.000028
C	-0.423742	-0.674143	0.000037
C	0.203061	0.519189	0.000064
S	1.946344	0.251141	0.000001
H	2.582275	-2.125915	0.000181
H	0.031548	-2.852687	0.000028
Cl	-0.463151	2.112279	0.000111

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1011.89818345 Predicted Change= -6.040665D-08
Zero-point correction (ZPE)= -1011.8532 0.04491
Internal Energy (U)= -1011.8480 0.05014
Enthalpy (H)= -1011.8470 0.05109
Gibbs Free Energy (G)= -1011.8835 0.01459

Frequencies -- 190.8973 254.3745 433.1403

Supporting Information: **2chloro4radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1011.90065516 Predicted Change= -6.085573D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00033	0.00180	[YES]	0.00033	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.940041	1.302689	0.000413
C	1.206607	-0.016604	0.000085
C	0.120706	-0.925790	-0.000177
C	-1.051954	-0.216621	-0.000011
S	-0.811059	1.514483	0.000258
H	1.591735	2.164816	0.000635
H	0.184917	-2.006139	-0.000412
Cl	-2.658090	-0.867707	-0.000166

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1011.90065516 Predicted Change= -6.085573D-08
Zero-point correction (ZPE)= -1011.8559 0.04472
Internal Energy (U)= -1011.8506 0.04996
Enthalpy (H)= -1011.8497 0.05090
Gibbs Free Energy (G)= -1011.8862 0.01444

Frequencies -- 207.4297 260.6375 430.1588

Supporting Information: **2chlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClS C1[X(C4H3ClS)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1012.59220856 Predicted Change= -2.025279D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00151	0.00180	[YES]	0.00151	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.021288	-0.204049	0.000078
C	-1.703945	1.124893	-0.000043
C	-0.295489	1.367784	0.000002
C	0.421625	0.204668	0.000013
S	-0.601420	-1.207547	-0.000032
H	-3.001259	-0.662113	0.000125
H	-2.447065	1.914896	-0.000077
H	0.162997	2.349556	-0.000017
Cl	2.147213	0.044626	0.000010

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1012.59220856 Predicted Change= -2.025279D-07
Zero-point correction (ZPE)= -1012.5346 0.05756
Internal Energy (U)= -1012.5294 0.06277
Enthalpy (H)= -1012.5284 0.06372
Gibbs Free Energy (G)= -1012.5642 0.02792

Frequencies -- 210.0651 260.3533 434.7620

Supporting Information: **3chloro2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1011.89698950 Predicted Change= -4.316640D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.720573	-1.469734	-0.000001
C	0.402001	-1.822591	0.000186
C	-0.474931	-0.681223	-0.000062
C	0.233394	0.473334	-0.000192
S	1.937639	0.269593	0.000124
H	2.587734	-2.117050	0.000029
H	0.040576	-2.844737	0.000327
Cl	-2.211371	-0.804942	-0.000196

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1011.89698950 Predicted Change= -4.316640D-08
Zero-point correction (ZPE)= -1011.8521 0.04481
Internal Energy (U)= -1011.8468 0.05010
Enthalpy (H)= -1011.8459 0.05105
Gibbs Free Energy (G)= -1011.8826 0.01437

Frequencies -- 162.0594 275.3256 402.1379

Supporting Information: **3chlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClS C1[X(C4H3ClS)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1012.59614893 Predicted Change= -1.422255D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00140	0.00180	[YES]	0.00140	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.444962	1.136062	0.000169
C	-0.088121	1.287865	-0.000107
C	0.583567	0.026563	0.000056
C	-0.253939	-1.052363	0.000109
S	-1.909540	-0.536785	-0.000082
H	-2.202276	1.908238	0.000237
H	0.425058	2.241814	-0.000223
H	0.006960	-2.100757	0.000152
Cl	2.326096	-0.108794	-0.000013

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1012.59614893 Predicted Change= -1.422255D-07
Zero-point correction (ZPE)= -1012.5386 0.05752
Internal Energy (U)= -1012.5334 0.06272
Enthalpy (H)= -1012.5324 0.06366
Gibbs Free Energy (G)= -1012.5682 0.02789

Frequencies -- 210.5948 284.1954 423.3276

Supporting Information: **4chloro2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1011.89983426 Predicted Change= -2.666655D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.916683	1.298550	0.000306
C	1.235922	-0.028863	0.000146
C	0.107507	-0.925927	-0.000297
C	-1.027218	-0.189861	-0.000300
S	-0.821405	1.515647	0.000384
H	1.583156	2.149773	0.000565
H	0.183901	-2.005541	-0.000602
Cl	2.881344	-0.614427	0.000263

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1011.89983426 Predicted Change= -2.666655D-08
Zero-point correction (ZPE)= -1011.8551 0.04472
Internal Energy (U)= -1011.8498 0.04998
Enthalpy (H)= -1011.8489 0.05092
Gibbs Free Energy (G)= -1011.8854 0.01440

Frequencies -- 202.2110 285.1718 360.2532

Chloropyrazines

Supporting Information: **2chloropyrazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -723.913976004 Predicted Change= -1.937329D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00039	0.00180	[YES]	0.00039	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.459147	-0.031645	0.000021
C	0.228850	1.190478	-0.000010
N	1.560564	1.220515	0.000011
C	2.191359	0.038300	0.000048
C	1.490087	-1.166027	0.000054
N	0.150021	-1.202059	0.000042
H	-0.304781	2.137035	-0.000062
H	3.278446	0.056386	0.000081
H	2.005360	-2.123675	0.000098
Cl	-2.215295	-0.022681	-0.000068

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -723.913976004 Predicted Change= -1.937329D-07

Zero-point correction (ZPE)= -723.8466 0.06733

Internal Energy (U)= -723.8413 0.07259

Enthalpy (H)= -723.8404 0.07353

Gibbs Free Energy (G)= -723.8763 0.03764

Frequencies -- 171.8395 306.4918 423.2547

Supporting Information: **2radicapyrazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -263.638180917 Predicted Change= -1.117172D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00119	0.00180	[YES]	0.00119	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.148842	-0.034842	0.000017
C	0.813300	1.197809	-0.000007
N	2.151016	1.211746	0.000027
C	2.784353	0.030433	0.000074
C	2.096687	-1.182493	0.000089
N	0.749582	-1.174917	0.000059
H	0.295003	2.151540	-0.000028
H	3.871721	0.054149	0.000091
H	2.608050	-2.141649	0.000117

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -263.638180917 Predicted Change= -1.117172D-06
Zero-point correction (ZPE)= -263.5740 0.06411
Internal Energy (U)= -263.5699 0.06827
Enthalpy (H)= -263.5689 0.06921
Gibbs Free Energy (G)= -263.6019 0.03619

Frequencies -- 364.4719 432.8125 570.8079

Bromopyrazines

Supporting Information: **2bromopyrazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN2 C1[X(C4H3BrN2)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -2835.42185695 Predicted Change= -3.618648D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00060	0.00180	[YES]	0.00060	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.139061	-0.029987	0.000029
C	0.827819	1.191073	0.000006
N	2.159868	1.218992	0.000029
C	2.788822	0.035683	0.000067
C	2.086208	-1.168038	0.000075
N	0.745624	-1.199800	0.000057
H	0.295604	2.138186	-0.000043
H	3.876005	0.052368	0.000099
H	2.599542	-2.126702	0.000118
Br	-1.776030	-0.010588	-0.000052

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2835.42185695 Predicted Change= -3.618648D-07

Zero-point correction (ZPE)= -2835.3550 0.06678

Internal Energy (U)= -2835.3495 0.07226

Enthalpy (H)= -2835.3486 0.07321

Gibbs Free Energy (G)= -2835.3858 0.03598

Frequencies -- 158.6920 257.4560 313.4093

Bromofurans

Supporting Information: **23dibromofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Br2O C1[X(C4H2Br2O)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -5372.21943201 Predicted Change= -1.334220D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00110	0.00180	[YES]	0.00110	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.663809	0.593880	0.000103
C	0.696836	0.673551	-0.000124
C	1.022578	2.068641	0.000394
C	-0.167712	2.723925	-0.000347
H	2.012217	2.501107	0.000710
H	-0.448246	3.765523	-0.000622
O	-1.210655	1.835864	0.000007
Br	1.891910	-0.770002	-0.000211
Br	-1.812084	-0.867527	0.000202

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5372.21943201 Predicted Change= -1.334220D-07

Zero-point correction (ZPE)= -5372.1690 0.05038

Internal Energy (U)= -5372.1627 0.05672

Enthalpy (H)= -5372.1617 0.05766

Gibbs Free Energy (G)= -5372.2022 0.01719

Frequencies -- 103.2501 185.0829 239.2894

Supporting Information: **24dibromofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Br2O C1[X(C4H2Br2O)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -5372.21952445 Predicted Change= -3.289675D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00117	0.00180	[YES]	0.00117	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.624683	1.479117	0.000335
C	-1.119472	0.212824	0.000168
C	-0.005699	-0.688038	0.000383
C	1.088521	0.120391	-0.000062
H	-1.072831	2.459103	0.000441
H	-0.027966	-1.766644	0.000555
O	0.744431	1.432515	0.000006
Br	-2.938457	-0.269887	0.000230
Br	2.913124	-0.270066	-0.000402

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5372.21952445 Predicted Change= -3.289675D-07
Zero-point correction (ZPE)= -5372.1691 0.05033
Internal Energy (U)= -5372.1628 0.05671
Enthalpy (H)= -5372.1618 0.05765
Gibbs Free Energy (G)= -5372.2024 0.01712

Frequencies -- 123.2061 142.2354 261.4655

Supporting Information: **2bromo3radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrO(2) C1[X(C4H2BrO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2800.41902137 Predicted Change= -1.036597D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00055	0.00180	[YES]	0.00055	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.661848	0.599568	0.000089
C	0.685264	0.690943	0.000351
C	1.056565	2.064965	0.000154
C	-0.134092	2.731022	-0.000104
H	2.047251	2.495329	0.000269
H	-0.400234	3.777196	-0.000290
O	-1.194018	1.861427	-0.000350
Br	-1.845316	-0.837820	0.000040

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2800.41902137 Predicted Change= -1.036597D-07
Zero-point correction (ZPE)= -2800.3714 0.04754
Internal Energy (U)= -2800.3665 0.05250
Enthalpy (H)= -2800.3655 0.05345
Gibbs Free Energy (G)= -2800.4019 0.01707

Frequencies -- 190.2037 259.2642 370.8948

Supporting Information: **2bromo4radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrO(2) C1[X(C4H2BrO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2800.42115463 Predicted Change= -1.239433D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00034	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00186	0.00180	[NO]	0.00186	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.636122	1.490713	0.000148
C	1.098721	0.222447	0.000433
C	0.012535	-0.696092	0.000167
C	-1.081442	0.121440	0.000343
H	1.071420	2.475930	0.000137
H	0.023522	-1.774886	0.000149
O	-0.746523	1.437408	0.000117
Br	-2.908770	-0.267664	0.000427

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2800.42115463 Predicted Change= -1.239433D-06
Zero-point correction (ZPE)= -2800.3735 0.04758
Internal Energy (U)= -2800.3686 0.05252
Enthalpy (H)= -2800.3676 0.05346
Gibbs Free Energy (G)= -2800.4040 0.01715

Frequencies -- 207.2380 263.4971 367.4281

Supporting Information: **2bromofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrO C1[X(C4H3BrO)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2801.11982369 Predicted Change= -4.596367D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00172	0.00180	[YES]	0.00172	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.333903	0.104841	-0.000124
C	-1.177545	1.172441	0.000378
C	-2.498851	0.611998	-0.000575
C	-2.344626	-0.739111	0.000644
H	-0.895404	2.214642	0.000752
H	-3.434698	1.153329	-0.000895
H	-3.026438	-1.575091	0.001212
O	-1.014601	-1.068491	-0.000429
Br	1.531511	-0.004170	0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2801.11982369 Predicted Change= -4.596367D-07
Zero-point correction (ZPE)= -2801.0595 0.06027
Internal Energy (U)= -2801.0545 0.06523
Enthalpy (H)= -2801.0536 0.06617
Gibbs Free Energy (G)= -2801.0893 0.03044

Frequencies -- 206.1472 261.4592 366.9162

Supporting Information: **2bromofuranradical2.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3O(2) C1[X(C4H3O)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -229.321276675 Predicted Change= -2.696304D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00024	0.00180	[YES]	0.00024	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.354318	0.096972	0.000260
C	-1.169591	1.182429	0.000054
C	-2.496541	0.608979	0.000000
C	-2.349642	-0.742980	0.000222
H	-0.891301	2.224804	-0.000058
H	-3.431811	1.152821	-0.000160
H	-3.028671	-1.581062	0.000293
O	-1.004191	-1.067404	0.000352

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -229.321276675 Predicted Change= -2.696304D-08
Zero-point correction (ZPE)= -229.2641 0.05715
Internal Energy (U)= -229.2603 0.06090
Enthalpy (H)= -229.2594 0.06184
Gibbs Free Energy (G)= -229.2909 0.03027

Frequencies -- 479.9989 606.0031 703.3667

Supporting Information: **3bromo2radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrO(2) C1[X(C4H2BrO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2800.41879474 Predicted Change= -1.069879D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00044	0.00180	[YES]	0.00044	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.641305	0.633405	-0.000124
C	0.715655	0.664397	0.000117
C	1.047476	2.068330	0.000003
C	-0.132661	2.742347	-0.000016
H	2.043236	2.488541	0.000065
H	-0.407369	3.785375	-0.000022
O	-1.188685	1.848155	-0.000275
Br	1.913509	-0.780373	0.000341

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2800.41879474 Predicted Change= -1.069879D-07
Zero-point correction (ZPE)= -2800.3714 0.04738
Internal Energy (U)= -2800.3663 0.05239
Enthalpy (H)= -2800.3654 0.05334
Gibbs Free Energy (G)= -2800.4019 0.01684

Frequencies -- 210.9622 249.4038 362.0162

Supporting Information: **3bromofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrO C1[X(C4H3BrO)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2801.12106801 Predicted Change= -1.567714D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00072	0.00180	[YES]	0.00072	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.117947	-1.097076	0.000271
C	0.316438	0.002262	-0.000035
C	1.170335	1.152320	0.000267
C	2.436959	0.657129	-0.000168
H	0.925556	-2.157851	0.000428
H	0.866684	2.188703	0.000467
H	3.413884	1.115719	-0.000324
O	2.423556	-0.706974	-0.000154
Br	-1.566990	0.006326	-0.000039

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2801.12106801 Predicted Change= -1.567714D-07
Zero-point correction (ZPE)= -2801.0605 0.06049
Internal Energy (U)= -2801.0556 0.06544
Enthalpy (H)= -2801.0546 0.06639
Gibbs Free Energy (G)= -2801.0904 0.03063

Frequencies -- 229.9232 248.2471 358.0740

Supporting Information: **3bromofuranradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3O(2) C1[X(C4H3O)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -229.321688687 Predicted Change= -2.024997D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00099	0.00180	[YES]	0.00099	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.107102	-1.106969	0.000338
C	0.335844	0.002805	-0.000163
C	1.162586	1.161819	0.000356
C	2.430835	0.656887	-0.000238
H	0.929057	-2.169629	0.000312
H	0.872139	2.202147	0.000518
H	3.408586	1.115429	-0.000473
O	2.425210	-0.708258	0.000101

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -229.321688687 Predicted Change= -2.024997D-07
Zero-point correction (ZPE)= -229.2641 0.05751
Internal Energy (U)= -229.2604 0.06121
Enthalpy (H)= -229.2595 0.06216
Gibbs Free Energy (G)= -229.2910 0.03067

Frequencies -- 546.0707 616.8968 695.5630

Supporting Information: **4bromo2radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrO(2) C1[X(C4H2BrO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2800.42191866 Predicted Change= -1.294524D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.635888	1.488393	-0.000053
C	1.124485	0.219303	0.000182
C	0.010524	-0.697889	0.000051
C	-1.060278	0.134800	0.000629
H	1.080184	2.470057	-0.000274
H	0.037197	-1.775497	-0.000102
O	-0.746198	1.429822	0.000738
Br	2.944568	-0.260949	-0.000064

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2800.42191866 Predicted Change= -1.294524D-07
Zero-point correction (ZPE)= -2800.3744 0.04746
Internal Energy (U)= -2800.3694 0.05243
Enthalpy (H)= -2800.3685 0.05337
Gibbs Free Energy (G)= -2800.4049 0.01698

Frequencies -- 229.9198 251.3845 358.8749

Bromoimidazoles

Supporting Information: **24dibromoimidazole.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt freq b3lyp/6-31g(d)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C3H2Br2N2   C1[X(C3H2Br2N2)]  #Atoms= 9
 Charge = 0     Multiplicity = 1
---------------------------------------------------------------------
 SCF Energy= -5368.41583877     Predicted Change= -3.463385D-08
=====================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00004 ||  0.00045   [ YES ]      0.00001 ||  0.00030   [ YES ]
 Displ      0.00038 ||  0.00180   [ YES ]      0.00038 ||  0.00180   [ YES ]
---------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
      Type       X           Y       Z
---------------------------------------------------------------------
      C        1.035598      0.204750      0.000004
      C       -1.074156      0.282942      0.000008
      C       -0.673646      1.594294      0.000255
      N        0.707851      1.527388      0.000105
      H        1.357892      2.300635      0.000136
      H       -1.218875      2.524324      0.000388
      N       -0.011276     -0.579501      0.000154
      Br       2.830207     -0.346797     -0.000071
      Br      -2.851402     -0.337548     -0.000042
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -5368.41583877 Predicted Change= -3.463385D-08
 Zero-point correction (ZPE)=        -5368.3647  0.05112
 Internal Energy (U)=               -5368.3583  0.05753
 Enthalpy (H)=                     -5368.3573   0.05848
 Gibbs Free Energy (G)=             -5368.3979    0.01793
---------------------------------------------------------------------
 Frequencies --   137.4600              141.3044              276.6536
```

Supporting Information: **25dibromoimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2Br2N2 C1[X(C3H2Br2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -5368.41438801 Predicted Change= -1.263072D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00090	0.00180	[YES]	0.00090	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.087518	0.365480	-0.000074
C	0.622457	1.641543	0.000014
C	1.102873	0.358855	0.000059
N	-0.004918	-0.466035	0.000051
H	-0.009179	-1.476053	0.000147
H	1.182778	2.564955	0.000025
N	-0.757928	1.628213	-0.000206
Br	-2.831682	-0.332388	-0.000177
Br	2.841381	-0.336738	0.000203

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5368.41438801 Predicted Change= -1.263072D-07
Zero-point correction (ZPE)= -5368.3631 0.05124
Internal Energy (U)= -5368.3566 0.05769
Enthalpy (H)= -5368.3557 0.05863
Gibbs Free Energy (G)= -5368.3964 0.01796

Frequencies -- 132.1211 133.0826 271.9169

Supporting Information: **2bromo4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrN2(2) C1[X(C3H2BrN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2796.62005219 Predicted Change= -5.291923D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00150	0.00180	[YES]	0.00150	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.036125	0.203877	0.000073
C	-1.057125	0.278617	0.000325
C	-0.683960	1.594627	0.000161
N	0.707806	1.526553	0.000177
H	1.364268	2.295403	0.000203
H	-1.223237	2.527671	0.000241
N	-0.024403	-0.574289	-0.000086
Br	2.834122	-0.344424	-0.000116

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2796.62005219 Predicted Change= -5.291923D-07
Zero-point correction (ZPE)= -2796.5714 0.04855
Internal Energy (U)= -2796.5665 0.05354
Enthalpy (H)= -2796.5655 0.05448
Gibbs Free Energy (G)= -2796.6019 0.01814

Frequencies -- 214.4029 271.4104 365.9792

Supporting Information: **2bromo5radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrN2(2) C1[X(C3H2BrN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2796.61584103 Predicted Change= -4.345425D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00033	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00119	0.00180	[YES]	0.00119	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.087378	0.354458	-0.000129
C	0.634993	1.650887	-0.000035
C	1.086271	0.363152	0.000051
N	-0.002397	-0.475595	0.000087
H	-0.004261	-1.484951	0.000171
H	1.182886	2.579852	-0.000037
N	-0.753300	1.618145	-0.000027
Br	-2.839932	-0.321379	-0.000243

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2796.61584103 Predicted Change= -4.345425D-07
Zero-point correction (ZPE)= -2796.5674 0.04840
Internal Energy (U)= -2796.5623 0.05347
Enthalpy (H)= -2796.5614 0.05441
Gibbs Free Energy (G)= -2796.5979 0.01791

Frequencies -- 205.0366 267.9542 363.8735

Supporting Information: **2bromoimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3BrN2 C1[X(C3H3BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2797.31523447 Predicted Change= -1.694301D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00100	0.00180	[YES]	0.00100	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.353635	-0.089286	0.000011
C	-2.384208	-0.716250	0.000065
C	-2.424292	0.654498	0.000203
N	-1.100082	1.052591	0.000131
H	-0.740873	1.996019	0.000226
H	-3.213936	-1.409292	0.000034
H	-3.235790	1.366219	0.000288
N	-1.080259	-1.173083	0.000071
Br	1.526451	-0.005808	-0.000104

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2797.31523447 Predicted Change= -1.694301D-07
Zero-point correction (ZPE)= -2797.2540 0.06121
Internal Energy (U)= -2797.2489 0.06624
Enthalpy (H)= -2797.2480 0.06718
Gibbs Free Energy (G)= -2797.2838 0.03137

Frequencies -- 212.5957 267.4274 363.8192

Supporting Information: **2bromoimidazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.520336906 Predicted Change= -2.362370D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00106	0.00180	[YES]	0.00106	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.362375	-0.095286	0.000360
C	-2.391914	-0.716611	-0.000205
C	-2.426514	0.652995	0.000552
N	-1.090202	1.052741	-0.000125
H	-0.736531	1.997156	-0.000323
H	-3.217627	-1.414345	-0.000499
H	-3.238822	1.365030	0.000794
N	-1.069091	-1.160264	0.000475

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.520336906 Predicted Change= -2.362370D-07
Zero-point correction (ZPE)= -225.4620 0.05827
Internal Energy (U)= -225.4582 0.06212
Enthalpy (H)= -225.4572 0.06306
Gibbs Free Energy (G)= -225.4889 0.03137

Frequencies -- 418.4776 582.9895 624.9386

Supporting Information: **45dibromoimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2Br2N2 C1[X(C3H2Br2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -5368.41522326 Predicted Change= -6.513772D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00161	0.00180	[YES]	0.00161	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.017732	2.694335	0.000163
C	-0.702138	0.675541	0.000140
C	0.668925	0.601975	-0.000050
N	1.101004	1.911189	0.000033
H	2.066723	2.208684	-0.000001
N	-1.120554	1.974077	-0.000026
Br	1.840543	-0.849351	-0.000219
H	0.030221	3.774538	0.000217
Br	-1.887813	-0.779540	0.000168

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5368.41522326 Predicted Change= -6.513772D-07
Zero-point correction (ZPE)= -5368.3638 0.05138
Internal Energy (U)= -5368.3574 0.05776
Enthalpy (H)= -5368.3565 0.05871
Gibbs Free Energy (G)= -5368.3970 0.01816

Frequencies -- 102.0889 187.3436 243.3005

Supporting Information: **4bromo2radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrN2(2) C1[X(C3H2BrN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2796.62132009 Predicted Change= -5.699196D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.022825	0.203636	-0.000037
C	-1.079913	0.283507	0.000132
C	-0.676092	1.593018	0.000091
N	0.716871	1.525383	0.000241
H	1.362546	2.300879	0.000380
H	-1.222700	2.523060	0.000143
N	0.004208	-0.574766	-0.000132
Br	-2.855759	-0.337434	0.000190

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2796.62132009 Predicted Change= -5.699196D-08
Zero-point correction (ZPE)= -2796.5729 0.04838
Internal Energy (U)= -2796.5678 0.05344
Enthalpy (H)= -2796.5669 0.05439
Gibbs Free Energy (G)= -2796.6034 0.01791

Frequencies -- 228.5309 270.3192 360.2303

Supporting Information: **4bromo5radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrN2(2) C1[X(C3H2BrN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2796.61418598 Predicted Change= -1.356071D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00053	0.00180	[YES]	0.00053	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.010932	2.697096	-0.000016
C	-0.701928	0.657291	0.000017
C	0.661712	0.617281	-0.000132
N	1.109820	1.913885	0.000111
H	2.074243	2.213604	0.000125
N	-1.110101	1.966745	0.000432
H	0.021862	3.777898	0.000012
Br	-1.906040	-0.783001	0.000096

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2796.61418598 Predicted Change= -1.356071D-07
Zero-point correction (ZPE)= -2796.5658 0.04838
Internal Energy (U)= -2796.5607 0.05346
Enthalpy (H)= -2796.5597 0.05441
Gibbs Free Energy (G)= -2796.5963 0.01785

Frequencies -- 204.8539 268.5452 363.6059

Supporting Information: **4bromoimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3BrN2 C1[X(C3H3BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2797.31643040 Predicted Change= -7.080222D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00036	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00185	0.00180	[NO]	0.00185	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.313371	-0.762392	-0.000089
C	0.332378	0.001138	-0.000002
C	1.137465	1.112189	0.000107
N	2.418939	0.599194	0.000074
H	3.273983	1.136962	0.000184
H	3.176250	-1.414197	-0.000171
H	0.921827	2.168461	0.000171
N	1.056061	-1.155696	0.000036
Br	-1.554181	-0.002895	-0.000030

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2797.31643040 Predicted Change= -7.080222D-07
Zero-point correction (ZPE)= -2797.2550 0.06134
Internal Energy (U)= -2797.2500 0.06635
Enthalpy (H)= -2797.2491 0.06729
Gibbs Free Energy (G)= -2797.2849 0.03152

Frequencies -- 228.7412 267.2396 358.8886

Supporting Information: **4bromoimidazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.520044563 Predicted Change= -3.998792D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00132	0.00180	[YES]	0.00132	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.316301	-0.762314	-0.000485
C	0.343843	-0.009574	0.000313
C	1.127004	1.114262	-0.000208
N	2.418772	0.598439	0.000497
H	3.277524	1.131997	0.000812
H	3.178820	-1.414931	-0.000782
H	0.920626	2.172078	-0.000380
N	1.047384	-1.144299	0.000543

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.520044563 Predicted Change= -3.998792D-07
Zero-point correction (ZPE)= -225.4614 0.05856
Internal Energy (U)= -225.4577 0.06230
Enthalpy (H)= -225.4567 0.06325
Gibbs Free Energy (G)= -225.4883 0.03173

Frequencies -- 524.1009 599.9792 671.2369

Supporting Information: **5bromo2radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrN2(2) C1[X(C3H2BrN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2796.62080926 Predicted Change= -7.317291D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00035	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00086	0.00180	[YES]	0.00086	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.080609	0.373493	0.000175
C	0.629747	1.645636	-0.000223
C	1.103148	0.360504	0.000278
N	-0.015103	-0.470141	-0.000152
H	-0.015039	-1.479226	-0.000266
H	1.186636	2.570903	-0.000403
N	-0.762145	1.610731	0.000248
Br	2.843312	-0.331680	0.000562

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2796.62080926 Predicted Change= -7.317291D-07
Zero-point correction (ZPE)= -2796.5722 0.04852
Internal Energy (U)= -2796.5671 0.05361
Enthalpy (H)= -2796.5662 0.05456
Gibbs Free Energy (G)= -2796.6028 0.01798

Frequencies -- 213.1079 252.1454 363.9655

Supporting Information: **5bromo4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrN2(2) C1[X(C3H2BrN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -2796.61799131 Predicted Change= -1.893118D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00077	0.00180	[YES]	0.00077	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.015213	2.697727	-0.000132
C	-0.704176	0.693861	0.000214
C	0.659058	0.592008	-0.000202
N	1.098776	1.909126	0.000281
H	2.064622	2.209269	0.000421
N	-1.117070	1.961060	0.000388
Br	1.849886	-0.850087	-0.000501
H	0.031109	3.778024	-0.000213

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2796.61799131 Predicted Change= -1.893118D-07
Zero-point correction (ZPE)= -2796.5692 0.04877
Internal Energy (U)= -2796.5642 0.05376
Enthalpy (H)= -2796.5632 0.05470
Gibbs Free Energy (G)= -2796.5996 0.01829

Frequencies -- 204.8625 255.0440 367.7196

Supporting Information: **5bromoimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3BrN2 C1[X(C3H3BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2797.31454511 Predicted Change= -2.034681D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00179	0.00180	[YES]	0.00179	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.412978	-0.621182	0.000218
C	1.200992	1.151137	0.000066
C	0.332324	0.090839	0.000025
N	1.112535	-1.044952	-0.000057
H	0.768856	-1.994666	-0.000162
H	3.245063	-1.312322	0.000296
H	0.963065	2.205064	0.000052
N	2.498714	0.691481	0.000185
Br	-1.540957	-0.004244	-0.000084

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2797.31454511 Predicted Change= -2.034681D-07
Zero-point correction (ZPE)= -2797.2530 0.06147
Internal Energy (U)= -2797.2480 0.06650
Enthalpy (H)= -2797.2470 0.06744
Gibbs Free Energy (G)= -2797.2829 0.03158

Frequencies -- 212.1837 249.6710 363.0582

Supporting Information: **5bromoimidazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -225.515272108 Predicted Change= -6.368329D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00125	0.00180	[YES]	0.00125	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.411281	-0.630026	0.000045
C	1.190782	1.164547	0.000026
C	0.347808	0.089422	-0.000226
N	1.109927	-1.052051	0.000053
H	0.767230	-2.001452	0.000030
H	3.252154	-1.310435	0.000116
H	0.965730	2.219686	0.000045
N	2.489615	0.685707	0.000535

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -225.515272108 Predicted Change= -6.368329D-07
Zero-point correction (ZPE)= -225.4568 0.05843
Internal Energy (U)= -225.4530 0.06223
Enthalpy (H)= -225.4520 0.06317
Gibbs Free Energy (G)= -225.4837 0.03155

Frequencies -- 434.4395 556.1786 679.1289

Bromothiazole

Supporting Information: **24dibromothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBr2NS C1[X(C3HBr2NS)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -5711.24624076 Predicted Change= -2.939020D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00079	0.00180	[YES]	0.00079	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.901880	1.590048	0.000194
C	-1.149564	0.249417	0.000325
C	1.020095	0.110336	0.000273
H	-1.606787	2.408279	0.000068
N	-0.066093	-0.590719	0.000114
S	0.817260	1.848410	0.000256
Br	2.749038	-0.634137	-0.000397
Br	-2.886713	-0.495766	0.000119

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5711.24624076 Predicted Change= -2.939020D-07

Zero-point correction (ZPE)= -5711.2112 0.03503

Internal Energy (U)= -5711.2045 0.04174

Enthalpy (H)= -5711.2035 0.04268

Gibbs Free Energy (G)= -5711.2451 0.00110

Frequencies -- 132.7824 142.1576 227.2364

Supporting Information: **25dibromothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBr2NS C1[X(C3HBr2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -5711.24368131 Predicted Change= -2.388869D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 ‖	0.00045	[YES]	0.00001 ‖	0.00030	[YES]
Displ	0.00030 ‖	0.00180	[YES]	0.00030 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.212998	0.267677	-0.000017
C	-0.632462	1.502326	0.000044
C	1.202758	0.299255	0.000295
H	-1.171002	2.441766	-0.000068
N	0.745806	1.506317	0.000110
S	0.006598	-0.981994	0.000072
Br	3.037196	-0.135853	0.000184
Br	-3.045738	-0.140993	-0.000292

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5711.24368131 Predicted Change= -2.388869D-08
Zero-point correction (ZPE)= -5711.2084 0.03527
Internal Energy (U)= -5711.2016 0.04203
Enthalpy (H)= -5711.2006 0.04298
Gibbs Free Energy (G)= -5711.2423 0.00129

Frequencies -- 89.6615 136.4250 238.4459

Supporting Information: **2bromo4radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBrNS(2) C1[X(C3HBrNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -3139.45601533 Predicted Change= -1.403193D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00016	0.00180	[YES]	0.00016	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.621943	-0.004647	0.000193
C	2.094337	1.239954	0.000245
C	0.187858	0.250479	-0.000051
H	3.646671	-0.344951	0.000278
N	0.766642	1.416706	0.000140
S	1.266074	-1.128444	0.000078
Br	-1.677005	-0.012331	-0.000138

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3139.45601533 Predicted Change= -1.403193D-08
Zero-point correction (ZPE)= -3139.4235 0.03249
Internal Energy (U)= -3139.4182 0.03773
Enthalpy (H)= -3139.4173 0.03868
Gibbs Free Energy (G)= -3139.4547 0.00126

Frequencies -- 198.8343 222.7794 336.7616

Supporting Information: **2bromo5radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBrNS(2) C1[X(C3HBrNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -3139.44949878 Predicted Change= -5.467955D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00144	0.00180	[YES]	0.00144	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.570739	-0.157115	0.000993
C	-2.213409	1.148349	-0.000211
C	-0.212482	0.198567	0.000721
H	-2.866382	2.010794	-0.000263
N	-0.833982	1.331951	-0.000575
S	-1.223836	-1.241377	-0.000372
Br	1.664726	0.039679	0.000035

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3139.44949878 Predicted Change= -5.467955D-07
Zero-point correction (ZPE)= -3139.4167 0.03270
Internal Energy (U)= -3139.4115 0.03795
Enthalpy (H)= -3139.4106 0.03889
Gibbs Free Energy (G)= -3139.4480 0.00142

Frequencies -- 200.3271 220.8150 334.3415

Supporting Information: **2bromothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNS C1[X(C3H2BrNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -3140.14649054 Predicted Change= -6.864528D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00144	0.00180	[YES]	0.00144	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.560947	-0.134687	0.000289
C	2.136752	1.161729	-0.000039
C	0.162931	0.218073	0.000002
H	3.572568	-0.516343	0.000436
H	2.785826	2.029696	0.000035
N	0.770904	1.356656	0.000526
S	1.189531	-1.202090	0.000022
Br	-1.712886	0.021509	-0.000172

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3140.14649054 Predicted Change= -6.864528D-07
Zero-point correction (ZPE)= -3140.1011 0.04529
Internal Energy (U)= -3140.0959 0.05054
Enthalpy (H)= -3140.0950 0.05148
Gibbs Free Energy (G)= -3140.1318 0.01467

Frequencies -- 198.6738 223.4568 334.0959

Supporting Information: **2bromothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.360798177 Predicted Change= -3.001141D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00030 ‖	0.00180	[YES]	0.00030 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.564594	-0.130836	0.000197
C	2.149162	1.165955	0.000118
C	0.163475	0.225585	0.000082
H	3.575581	-0.515845	0.000303
H	2.788756	2.040016	0.000190
N	0.764886	1.330846	0.000212
S	1.173006	-1.202688	0.000169

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.360798177 Predicted Change= -3.001141D-08
Zero-point correction (ZPE)= -568.3181 0.04263
Internal Energy (U)= -568.3141 0.04660
Enthalpy (H)= -568.3132 0.04754
Gibbs Free Energy (G)= -568.3459 0.01485

Frequencies -- 438.1695 551.6810 569.8103

Supporting Information: **4bromo2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBrNS(2) C1[X(C3HBrNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -3139.46035855 Predicted Change= -2.278317D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00105	0.00180	[YES]	0.00105	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.906516	-0.995771	0.000406
C	-0.061679	0.072593	0.000121
C	-1.921698	1.203394	0.000545
H	-0.662984	-2.048478	0.000386
N	-0.666105	1.319924	0.000335
S	-2.564677	-0.419501	-0.000321
Br	1.819998	-0.061722	-0.000115

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3139.46035855 Predicted Change= -2.278317D-07
Zero-point correction (ZPE)= -3139.4277 0.03259
Internal Energy (U)= -3139.4224 0.03786
Enthalpy (H)= -3139.4215 0.03880
Gibbs Free Energy (G)= -3139.4590 0.00133

Frequencies -- 188.4845 250.6941 324.1134

Supporting Information: **4bromothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNS C1[X(C3H2BrNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -3140.14762967 Predicted Change= -4.339951D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019 ‖	0.00045	[YES]	0.00006 ‖	0.00030	[YES]
Displ	0.00211 ‖	0.00180	[NO]	0.00211 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.853252	-1.039486	-0.000029
C	0.039487	0.056218	0.000120
C	1.935699	1.137904	0.000166
H	0.581271	-2.084245	-0.000136
N	0.642497	1.283671	-0.000066
S	2.504523	-0.513422	0.000028
H	2.634018	1.966466	0.000215
Br	-1.850165	-0.045171	-0.000046

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3140.14762967 Predicted Change= -4.339951D-07
Zero-point correction (ZPE)= -3140.1023 0.04529
Internal Energy (U)= -3140.0971 0.05051
Enthalpy (H)= -3140.0961 0.05145
Gibbs Free Energy (G)= -3140.1329 0.01469

Frequencies -- 189.5206 251.2723 324.7948

Supporting Information: **4bromothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.356726189 Predicted Change= -8.040025D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00036	0.00180	[YES]	0.00036	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.835659	-1.047856	-0.000084
C	0.065317	0.065727	0.000052
C	1.938786	1.143323	0.000104
H	0.574513	-2.095242	-0.000147
N	0.634952	1.273739	0.000098
S	2.506729	-0.506878	0.000138
H	2.634791	1.974293	0.000137

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.356726189 Predicted Change= -8.040025D-08
Zero-point correction (ZPE)= -568.3141 0.04256
Internal Energy (U)= -568.3102 0.04646
Enthalpy (H)= -568.3093 0.04741
Gibbs Free Energy (G)= -568.3418 0.01483

Frequencies -- 458.9562 596.2855 613.2142

Supporting Information: **5bromo2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBrNS(2) C1[X(C3HBrNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -3139.45918509 Predicted Change= -2.892903D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00159	0.00180	[YES]	0.00159	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.189216	0.190638	-0.000117
C	0.918047	1.342397	0.000667
C	2.591247	-0.095688	-0.000917
H	0.519331	2.348402	0.001155
N	2.292591	1.127062	-0.000179
S	1.251304	-1.217851	0.000359
Br	-1.679411	0.017820	-0.000099

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3139.45918509 Predicted Change= -2.892903D-07
Zero-point correction (ZPE)= -3139.4263 0.03279
Internal Energy (U)= -3139.4210 0.03810
Enthalpy (H)= -3139.4201 0.03904
Gibbs Free Energy (G)= -3139.4577 0.00146

Frequencies -- 205.5727 207.4290 331.3017

Supporting Information: **5bromothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNS C1[X(C3H2BrNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -3140.14406672 Predicted Change= -7.353351D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00024	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00125	0.00180	[YES]	0.00125	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.146888	0.187873	-0.000033
C	0.875605	1.342973	-0.000270
C	2.553161	-0.087276	0.000003
H	0.451382	2.339741	-0.000262
N	2.240111	1.174900	0.000642
S	1.200572	-1.198268	-0.000006
H	3.571032	-0.460276	0.000033
Br	-1.724751	0.011632	-0.000068

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3140.14406672 Predicted Change= -7.353351D-07
Zero-point correction (ZPE)= -3140.0985 0.04549
Internal Energy (U)= -3140.0933 0.05075
Enthalpy (H)= -3140.0923 0.05169
Gibbs Free Energy (G)= -3140.1292 0.01482

Frequencies -- 199.0845 211.0753 330.3012

Supporting Information: **5bromothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.349202571 Predicted Change= -8.997638D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00039	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00198	0.00180	[NO]	0.00198	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.175056	0.183859	-0.000246
C	0.860113	1.352945	0.000077
C	2.551720	-0.093903	0.000126
H	0.449434	2.353865	-0.000129
N	2.235704	1.169728	0.000085
S	1.193973	-1.209083	-0.000013
H	3.572751	-0.457745	0.000208

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.349202571 Predicted Change= -8.997638D-07
Zero-point correction (ZPE)= -568.3064 0.04274
Internal Energy (U)= -568.3025 0.04665
Enthalpy (H)= -568.3016 0.04760
Gibbs Free Energy (G)= -568.3342 0.01498

Frequencies -- 416.3373 582.0011 591.1636

Bromoisothiazoles

Supporting Information: **35dibromoisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBr2NS C1[X(C3HBr2NS)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -5711.24129875 Predicted Change= -2.317945D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00179	0.00180	[YES]	0.00179	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.175374	0.210853	0.000109
C	0.056664	-0.674599	0.000105
C	-1.087858	0.072904	-0.000015
S	-0.698758	1.761341	0.000141
H	0.112998	-1.754059	0.000118
N	0.964108	1.500086	-0.000035
Br	2.958754	-0.441549	0.000034
Br	-2.860089	-0.546536	-0.000129

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5711.24129875 Predicted Change= -2.317945D-07

Zero-point correction (ZPE)= -5711.2061 0.03512

Internal Energy (U)= -5711.1994 0.04182

Enthalpy (H)= -5711.1985 0.04276

Gibbs Free Energy (G)= -5711.2401 0.00118

Frequencies -- 129.2125 132.9751 248.5511

Supporting Information: **3bromo5radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBrNS(2) C1[X(C3HBrNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -3139.44861392 Predicted Change= -3.874606D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00117	0.00180	[YES]	0.00117	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.172222	0.203042	-0.000345
C	0.052064	-0.688506	-0.000148
C	-1.058427	0.095551	0.000701
S	-0.714233	1.765099	-0.000550
H	0.102747	-1.768240	0.000068
N	0.965609	1.496559	0.000640
Br	2.961300	-0.428527	0.000091

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3139.44861392 Predicted Change= -3.874606D-07
Zero-point correction (ZPE)= -3139.4159 0.03262
Internal Energy (U)= -3139.4107 0.03781
Enthalpy (H)= -3139.4098 0.03876
Gibbs Free Energy (G)= -3139.4471 0.00144

Frequencies -- 203.9341 251.5173 319.5934

Supporting Information: **3bromoisothiazole2.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNS C1[X(C3H2BrNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -3140.14337328 Predicted Change= -1.212598D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00046	0.00180	[YES]	0.00046	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.062325	0.056508	-0.000005
C	0.742616	1.312090	0.000079
C	2.091187	1.092560	-0.000014
S	2.395828	-0.606610	-0.000054
H	0.251835	2.276177	0.000095
H	2.889178	1.824277	-0.000072
N	0.769794	-1.040874	0.000160
Br	-1.835417	-0.053587	-0.000019

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3140.14337328 Predicted Change= -1.212598D-07
Zero-point correction (ZPE)= -3140.0981 0.04517
Internal Energy (U)= -3140.0929 0.05038
Enthalpy (H)= -3140.0920 0.05133
Gibbs Free Energy (G)= -3140.1287 0.01460

Frequencies -- 199.6148 253.0668 320.2384

Supporting Information: **3bromoisothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.356792065 Predicted Change= -7.293026D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00130	0.00180	[YES]	0.00130	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.086644	0.047959	-0.000002
C	0.735646	1.317604	0.000158
C	2.086979	1.090816	-0.000118
S	2.422623	-0.608841	0.000258
H	0.250001	2.283817	0.000201
H	2.885135	1.823808	-0.000232
N	0.735736	-1.041035	-0.000076

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.356792065 Predicted Change= -7.293026D-07
Zero-point correction (ZPE)= -568.3145 0.04225
Internal Energy (U)= -568.3105 0.04624
Enthalpy (H)= -568.3096 0.04718
Gibbs Free Energy (G)= -568.3423 0.01448

Frequencies -- 453.3436 530.9961 576.4957

Supporting Information: **4bromoisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNS C1[X(C3H2BrNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -3140.14123357 Predicted Change= -4.412135D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00300	0.00180	[NO]	0.00300	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.766276	1.251794	0.000025
C	-0.027869	0.030312	0.000031
C	-0.860020	-1.054891	0.000188
S	-2.486815	-0.489609	-0.000103
H	-0.315661	2.239830	-0.000020
H	-0.595467	-2.103479	0.000274
N	-2.075963	1.142878	0.000097
Br	1.861626	-0.047601	-0.000022

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3140.14123357 Predicted Change= -4.412135D-07
Zero-point correction (ZPE)= -3140.0958 0.04538
Internal Energy (U)= -3140.0906 0.05060
Enthalpy (H)= -3140.0896 0.05154
Gibbs Free Energy (G)= -3140.1264 0.01476

Frequencies -- 197.0318 236.2905 321.0358

Supporting Information: **4bromoisothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.346962529 Predicted Change= -6.172710D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00143	0.00180	[YES]	0.00143	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.756449	1.262543	-0.000016
C	-0.057754	0.030087	0.000121
C	-0.847956	-1.068756	0.000136
S	-2.487778	-0.489902	0.000007
H	-0.314501	2.253176	0.000004
H	-0.591208	-2.119411	0.000230
N	-2.072425	1.149097	0.000009

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.346962529 Predicted Change= -6.172710D-07
Zero-point correction (ZPE)= -568.3043 0.04261
Internal Energy (U)= -568.3004 0.04649
Enthalpy (H)= -568.2995 0.04743
Gibbs Free Energy (G)= -568.3320 0.01490

Frequencies -- 460.1075 571.7673 619.8656

Supporting Information: **5bromo3radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3HBrNS(2) C1[X(C3HBrNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -3139.45582221 Predicted Change= -1.578645D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00059	0.00180	[YES]	0.00059	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.154852	0.227847	0.000112
C	0.061836	-0.683537	0.000049
C	-1.081651	0.072356	0.000036
S	-0.721788	1.774476	-0.000062
H	0.113367	-1.762864	0.000049
N	0.992429	1.486477	0.000138
Br	-2.856606	-0.544765	-0.000027

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3139.45582221 Predicted Change= -1.578645D-07
Zero-point correction (ZPE)= -3139.4234 0.03237
Internal Energy (U)= -3139.4181 0.03770
Enthalpy (H)= -3139.4171 0.03864
Gibbs Free Energy (G)= -3139.4547 0.00106

Frequencies -- 202.0397 207.8287 330.6706

Supporting Information: **5bromoisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNS C1[X(C3H2BrNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -3140.13901885 Predicted Change= -1.833729D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00131	0.00180	[YES]	0.00131	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.257950	1.041430	0.000191
C	-0.868458	1.355405	0.000053
C	-0.140284	0.195384	-0.000055
S	-1.205140	-1.168027	0.000160
H	-3.053045	1.782596	0.000221
H	-0.446306	2.352165	0.000132
N	-2.600518	-0.232068	-0.000450
Br	1.731011	0.017852	-0.000026

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3140.13901885 Predicted Change= -1.833729D-07
Zero-point correction (ZPE)= -3140.0936 0.04538
Internal Energy (U)= -3140.0883 0.05062
Enthalpy (H)= -3140.0874 0.05156
Gibbs Free Energy (G)= -3140.1242 0.01473

Frequencies -- 200.3325 207.1558 333.2966

Supporting Information: **5bromoisothiazoleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -568.345614613 Predicted Change= -3.627959D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00059	0.00180	[YES]	0.00059	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.254235	1.044725	-0.000034
C	-0.861327	1.364787	0.000045
C	-0.174702	0.187841	0.000198
S	-1.189059	-1.179199	-0.000341
H	-3.055882	1.779303	0.000031
H	-0.437394	2.360843	0.000173
N	-2.599101	-0.231415	0.000179

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -568.345614613 Predicted Change= -3.627959D-07
Zero-point correction (ZPE)= -568.3029 0.04268
Internal Energy (U)= -568.2990 0.04656
Enthalpy (H)= -568.2981 0.04751
Gibbs Free Energy (G)= -568.3306 0.01496

Frequencies -- 434.5454 586.4190 611.3530

Bromoisoxazoles

Supporting Information: **3bromoisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -705.625326811 Predicted Change= -1.885277D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00099	0.00180	[YES]	0.00099	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.846532	0.591647	0.000019
C	-0.609007	1.150837	0.000027
C	0.240395	0.008186	-0.000033
H	-2.848566	0.996867	-0.000022
H	-0.326345	2.191586	0.000003
N	-0.413497	-1.129232	0.000234
O	-1.758685	-0.752195	-0.000059
Cl	1.966455	0.013512	-0.000073

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.625326811 Predicted Change= -1.885277D-07

Zero-point correction (ZPE)= -705.5766 0.04869

Internal Energy (U)= -705.5720 0.05328

Enthalpy (H)= -705.5710 0.05423

Gibbs Free Energy (G)= -705.6052 0.02008

Frequencies -- 258.8084 313.7286 488.2311

Supporting Information: **4bromoisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -705.622973921 Predicted Change= -1.166850D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 ‖	0.00045	[YES]	0.00001 ‖	0.00030	[YES]
Displ	0.00021 ‖	0.00180	[YES]	0.00021 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.564573	-1.086214	0.000008
C	-0.270205	-0.010992	-0.000012
C	0.608347	1.108612	0.000054
H	0.402400	-2.153820	0.000003
N	1.865276	0.736508	-0.000003
H	0.356299	2.161037	0.000069
O	1.839790	-0.663035	0.000080
Cl	-1.997074	0.004298	-0.000058

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.622973921 Predicted Change= -1.166850D-08
Zero-point correction (ZPE)= -705.5741 0.04879
Internal Energy (U)= -705.5695 0.05341
Enthalpy (H)= -705.5686 0.05435
Gibbs Free Energy (G)= -705.6028 0.02009

Frequencies -- 255.9066 290.1389 482.7155

Supporting Information: **5bromoisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -705.624900368 Predicted Change= -6.566954D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.233558	0.097069	-0.000012
C	0.617847	1.159969	-0.000078
C	1.890486	0.528082	0.000113
H	0.374835	2.210633	-0.000133
N	1.811727	-0.783135	-0.000136
H	2.870458	0.989373	0.000173
O	0.434178	-1.065753	0.000096
Cl	-1.944086	0.005720	0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.624900368 Predicted Change= -6.566954D-08
Zero-point correction (ZPE)= -705.5762 0.04867
Internal Energy (U)= -705.5716 0.05327
Enthalpy (H)= -705.5706 0.05422
Gibbs Free Energy (G)= -705.6048 0.02003

Frequencies -- 235.4618 309.7176 493.1690

Bromopyrazoles

Supporting Information: **3bromopyrazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3BrN2 C1[X(C3H3BrN2)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -2797.29971329 Predicted Change= -1.986769D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.439812	0.649055	0.000040
C	1.159071	1.164575	0.000080
C	0.336184	0.016646	-0.000005
N	2.307916	-0.703030	-0.000008
H	3.037323	-1.400122	-0.000092
H	3.407897	1.129505	0.000078
H	0.854442	2.199426	0.000147
Br	-1.549087	-0.004570	-0.000014
N	1.021793	-1.118471	-0.000039

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2797.29971329 Predicted Change= -1.986769D-07

Zero-point correction (ZPE)= -2797.2383 0.06137

Internal Energy (U)= -2797.2333 0.06637

Enthalpy (H)= -2797.2323 0.06731

Gibbs Free Energy (G)= -2797.2681 0.03155

Frequencies -- 232.5142 267.2021 361.1142

Supporting Information: **4bromopyrazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3BrN2 C1[X(C3H3BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2797.29884363 Predicted Change= -4.647472D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00287	0.00180	[NO]	0.00287	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.147353	-1.098676	0.000103
C	0.314484	0.002481	0.000015
C	1.168966	1.126364	0.000140
N	2.407060	-0.592894	0.000130
H	3.276874	-1.104593	0.000228
H	0.936957	-2.157545	0.000107
N	2.448045	0.756615	0.000016
H	0.897967	2.172895	0.000161
Br	-1.568067	-0.006795	-0.000088

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2797.29884363 Predicted Change= -4.647472D-07
Zero-point correction (ZPE)= -2797.2371 0.06166
Internal Energy (U)= -2797.2321 0.06666
Enthalpy (H)= -2797.2312 0.06761
Gibbs Free Energy (G)= -2797.2670 0.03178

Frequencies -- 230.5690 246.6880 360.2236

Supporting Information: **5bromopyrazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H3BrN2 C1[X(C3H3BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -2797.29868277 Predicted Change= -1.667967D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00075	0.00180	[YES]	0.00075	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.336076	0.091012	0.000003
C	1.197693	1.168347	-0.000096
C	2.478666	0.571088	0.000087
N	1.096809	-1.032120	0.000054
H	0.776321	-1.989297	0.000153
H	0.934937	2.214909	-0.000183
N	2.419868	-0.761116	-0.000039
H	3.443499	1.061027	0.000135
Br	-1.538460	0.008095	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2797.29868277 Predicted Change= -1.667967D-07
Zero-point correction (ZPE)= -2797.2371 0.06152
Internal Energy (U)= -2797.2321 0.06653
Enthalpy (H)= -2797.2312 0.06747
Gibbs Free Energy (G)= -2797.2670 0.03165

Frequencies -- 218.3256 250.4084 364.0731

Supporting Information: **3bromopyridazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN2 C1[X(C4H3BrN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2835.39052316 Predicted Change= -9.007250D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00066	0.00180	[YES]	0.00066	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.719549	-1.192695	-0.000010
C	-0.139486	-0.004677	-0.000019
C	-0.819827	1.219899	-0.000003
C	-2.199456	1.143001	0.000006
C	-2.770641	-0.136357	0.000006
N	-2.058019	-1.263050	0.000001
H	-0.281534	2.160891	0.000002
H	-2.819783	2.034340	0.000013
H	-3.848382	-0.275990	0.000011
Br	1.770547	-0.001721	0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2835.39052316 Predicted Change= -9.007250D-08
Zero-point correction (ZPE)= -2835.3244 0.06604
Internal Energy (U)= -2835.3189 0.07158
Enthalpy (H)= -2835.3179 0.07252
Gibbs Free Energy (G)= -2835.3552 0.03523

Frequencies -- 163.4262 261.0699 318.1479

Bromopyridazines

Supporting Information: 3 **radicalpyridazine.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C4H3N2(2)   C1[X(C4H3N2)]  #Atoms= 9
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -263.606126723     Predicted Change= -1.012490D-06
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00031 ||  0.00045   [ YES ]      0.00010 ||  0.00030   [ YES ]
 Displ      0.00158 ||  0.00180   [ YES ]      0.00158 ||  0.00180   [ YES ]
---------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
       Type      X           Y      Z
---------------------------------------------------------------------
       N       -0.721036     -1.162306     -0.000012
       C       -0.162457     -0.012117     -0.000011
       C       -0.805385      1.229013     -0.000002
       C       -2.187689      1.137415      0.000007
       C       -2.765504     -0.146972      0.000006
       N       -2.076023     -1.285550     -0.000003
       H       -0.274050      2.175025     -0.000003
       H       -2.818802      2.022498      0.000014
       H       -3.845731     -0.271643      0.000012
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -263.606126723 Predicted Change= -1.012490D-06
 Zero-point correction (ZPE)=         -263.5430  0.06307
 Internal Energy (U)=                 -263.5387  0.06734
 Enthalpy (H)=                        -263.5378   0.06829
 Gibbs Free Energy (G)=               -263.5710    0.03508
---------------------------------------------------------------------
 Frequencies --   352.1354              406.4568              554.2225
```

Supporting Information: **4bromopyridazine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN2 C1[X(C4H3BrN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2835.39071101 Predicted Change= -8.429398D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00053	0.00180	[YES]	0.00053	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-2.165942	-1.212715	-0.000001
C	-0.831872	-1.174184	-0.000002
C	-0.110233	0.024134	0.000000
C	-0.823003	1.207676	0.000003
C	-2.217541	1.087240	0.000004
N	-2.868507	-0.078233	0.000001
H	-0.328146	-2.136435	-0.000005
H	-0.336569	2.176953	0.000005
H	-2.850022	1.971601	0.000006
Br	1.790051	0.004438	-0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2835.39071101 Predicted Change= -8.429398D-08
Zero-point correction (ZPE)= -2835.3244 0.06631
Internal Energy (U)= -2835.3188 0.07183
Enthalpy (H)= -2835.3179 0.07277
Gibbs Free Energy (G)= -2835.3552 0.03547

Frequencies -- 167.5619 247.1045 314.8327

Supporting Information: **4radicalpyridazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -263.603220839 Predicted Change= -6.438577D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00039	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00105	0.00180	[YES]	0.00105	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
N	-2.162488	-1.199327	-0.000001
C	-0.808316	-1.184009	-0.000001
C	-0.136157	0.021192	0.000000
C	-0.817076	1.207970	0.000003
C	-2.222271	1.096343	0.000004
N	-2.851632	-0.078950	0.000001
H	-0.332963	-2.159462	-0.000005
H	-0.340631	2.184828	0.000005
H	-2.860301	1.977453	0.000006

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -263.603220839 Predicted Change= -6.438577D-07
Zero-point correction (ZPE)= -263.5400 0.06316
Internal Energy (U)= -263.5358 0.06735
Enthalpy (H)= -263.5349 0.06829
Gibbs Free Energy (G)= -263.5680 0.03521

Frequencies -- 374.2632 417.2313 599.0696

Bromopyridines

Supporting Information: **23dibromopyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3Br2N C1[X(C5H3Br2N)] #Atoms= 11

Charge = 0 Multiplicity = 1

SCF Energy= -5390.49072273 Predicted Change= -2.183283D-05

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00040	0.00045	[YES]	0.00019	0.00030	[YES]
Displ	0.02859	0.00180	[NO]	0.02859	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.616199	0.667823	0.000887
C	0.514294	-0.732566	0.000510
C	1.695003	-1.472644	0.007920
C	2.917010	-0.802292	0.000574
C	2.903852	0.590164	-0.007446
N	1.771500	1.304004	-0.000686
H	1.646291	-2.556082	0.025245
H	3.852372	-1.352824	-0.002364
H	3.827484	1.163914	-0.007006
Br	-0.953709	1.760404	0.001102
Br	-1.149285	-1.642860	-0.001838

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5390.49072273 Predicted Change= -2.183283D-05

Zero-point correction (ZPE)= -5390.4221 0.06860

Internal Energy (U)= -5390.4151 0.07558

Enthalpy (H)= -5390.4141 0.07652

Gibbs Free Energy (G)= -5390.4560 0.03468

Frequencies -- 109.8182 133.3247 230.8723

Supporting Information: **24dibromopyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3Br2N C1[X(C5H3Br2N)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -5390.49361714 Predicted Change= -2.993690D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00112	0.00180	[YES]	0.00112	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.179376	0.353919	-0.000007
C	-0.000594	-0.395444	0.000001
C	-1.189721	0.325398	-0.000009
C	-1.166407	1.719720	0.000002
C	0.081989	2.338055	0.000009
N	1.245356	1.671078	-0.000007
H	0.014943	-1.477235	0.000012
H	-2.081052	2.300445	0.000009
H	0.155268	3.423240	0.000001
Br	2.845031	-0.598550	0.000001
Br	-2.851731	-0.601276	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5390.49361714 Predicted Change= -2.993690D-07
Zero-point correction (ZPE)= -5390.4250 0.06861
Internal Energy (U)= -5390.4180 0.07561
Enthalpy (H)= -5390.4170 0.07655
Gibbs Free Energy (G)= -5390.4591 0.03449

Frequencies -- 133.2761 141.1127 190.5185

Supporting Information: **25dibromopyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3Br2N C1[X(C5H3Br2N)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -5390.49282725 Predicted Change= -2.616026D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00068	0.00180	[YES]	0.00068	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.340116	0.005787	-0.000199
C	-0.702061	1.249137	-0.000114
C	0.689595	1.256481	0.000075
C	1.359583	0.033093	0.000187
C	0.622587	-1.149989	0.000115
N	-0.715895	-1.156377	-0.000087
H	1.241059	2.190774	0.000130
H	-1.272810	2.170335	-0.000198
H	1.118750	-2.116667	0.000181
Br	-3.257230	-0.039275	-0.000441
Br	3.261423	-0.032635	0.000444

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5390.49282725 Predicted Change= -2.616026D-07
Zero-point correction (ZPE)= -5390.4242 0.06861
Internal Energy (U)= -5390.4171 0.07564
Enthalpy (H)= -5390.4162 0.07658
Gibbs Free Energy (G)= -5390.4583 0.03449

Frequencies -- 74.7035 165.8497 214.7240

Supporting Information: **2bromo3radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3BrN(2) C1[X(C5H3BrN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -2818.70108415 Predicted Change= -3.669131D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00116	0.00180	[YES]	0.00116	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.619589	0.683724	0.001687
C	0.556722	-0.691255	0.008889
C	1.681926	-1.480662	0.009626
C	2.915440	-0.807201	0.002395
C	2.903002	0.587705	-0.004500
N	1.781285	1.323026	-0.005334
H	1.629013	-2.566317	0.014955
H	3.854473	-1.353262	0.002063
H	3.833176	1.151096	-0.010983
Br	-0.984329	1.723047	-0.000061

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2818.70108415 Predicted Change= -3.669131D-07
Zero-point correction (ZPE)= -2818.6353 0.06576
Internal Energy (U)= -2818.6297 0.07133
Enthalpy (H)= -2818.6288 0.07227
Gibbs Free Energy (G)= -2818.6667 0.03432

Frequencies -- 165.3530 248.6943 313.4093

Supporting Information: **2bromo4radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3BrN(2) C1[X(C5H3BrN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -2818.70387803 Predicted Change= -2.102449D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00098	0.00180	[YES]	0.00098	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.178236	0.348282	0.000006
C	-0.007151	-0.411164	0.000001
C	-1.151136	0.346823	0.000003
C	-1.180877	1.723997	0.000003
C	0.078547	2.341791	-0.000003
N	1.234304	1.664727	0.000001
H	0.013670	-1.494795	0.000000
H	-2.094479	2.309697	0.000006
H	0.159340	3.427487	-0.000001
Br	2.853734	-0.596218	-0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2818.70387803 Predicted Change= -2.102449D-07
Zero-point correction (ZPE)= -2818.6383 0.06557
Internal Energy (U)= -2818.6327 0.07113
Enthalpy (H)= -2818.6317 0.07208
Gibbs Free Energy (G)= -2818.6697 0.03415

Frequencies -- 159.8333 264.5545 309.0655

Supporting Information: **2bromo5radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3BrN(2) C1[X(C5H3BrN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -2818.70092136 Predicted Change= -1.002202D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.331070	0.007142	-0.000197
C	-0.702381	1.257454	-0.000109
C	0.696969	1.263952	0.000073
C	1.320778	0.033604	0.000179
C	0.637111	-1.162244	0.000149
N	-0.713797	-1.157923	-0.000078
H	1.248011	2.200759	0.000125
H	-1.280685	2.174814	-0.000198
H	1.121448	-2.134326	0.000156
Br	-3.252922	-0.039933	-0.000451

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2818.70092136 Predicted Change= -1.002202D-07
Zero-point correction (ZPE)= -2818.6351 0.06576
Internal Energy (U)= -2818.6295 0.07133
Enthalpy (H)= -2818.6286 0.07227
Gibbs Free Energy (G)= -2818.6665 0.03434

Frequencies -- 174.8934 260.7968 312.0977

Supporting Information: **2bromopyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4BrN C1[X(C5H4BrN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -2819.39074384 Predicted Change= -1.983810D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00056	0.00180	[YES]	0.00056	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.133472	-0.015363	-0.000018
C	0.799322	1.213140	0.000091
C	2.191340	1.178990	0.000295
C	2.842180	-0.056834	0.000415
C	2.062775	-1.211414	0.000349
N	0.720765	-1.195209	0.000113
H	2.757505	2.106386	0.000359
H	0.246417	2.145085	0.000003
H	3.925395	-0.125069	0.000561
H	2.523249	-2.197060	0.000401
Br	-1.790642	-0.006114	-0.000254

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2819.39074384 Predicted Change= -1.983810D-07
Zero-point correction (ZPE)= -2819.3119 0.07879
Internal Energy (U)= -2819.3063 0.08438
Enthalpy (H)= -2819.3054 0.08533
Gibbs Free Energy (G)= -2819.3427 0.04796

Frequencies -- 162.0978 261.9157 309.3662

Supporting Information: **3bromo2radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3BrN(2) C1[X(C5H3BrN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -2818.70799774 Predicted Change= -2.861610D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00121	0.00180	[YES]	0.00121	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.639133	0.636478	-0.003710
C	0.512034	-0.744786	0.002603
C	1.696220	-1.481400	0.006103
C	2.916725	-0.793550	0.002989
C	2.914121	0.598178	-0.003828
N	1.750377	1.282313	-0.006934
H	1.665946	-2.566953	0.011131
H	3.854970	-1.339659	0.005888
H	3.832829	1.177990	-0.006548
Br	-1.187635	-1.601975	0.008102

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2818.70799774 Predicted Change= -2.861610D-07
Zero-point correction (ZPE)= -2818.6419 0.06603
Internal Energy (U)= -2818.6363 0.07160
Enthalpy (H)= -2818.6354 0.07255
Gibbs Free Energy (G)= -2818.6734 0.03457

Frequencies -- 171.8949 244.5095 319.2238

Supporting Information: **3bromopyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4BrN C1[X(C5H4BrN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -2819.38859374 Predicted Change= -3.799676D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00036	0.00180	[YES]	0.00036	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.811869	-1.192560	-0.000048
C	0.111842	0.015544	0.000011
C	0.811151	1.219034	0.000235
C	2.204052	1.159371	0.000385
C	2.821695	-0.092117	0.000282
N	2.146864	-1.248311	0.000083
H	0.283342	2.167009	0.000285
H	0.275950	-2.138803	-0.000231
H	2.797630	2.068810	0.000580
H	3.906934	-0.172605	0.000416
Br	-1.795873	0.004518	-0.000195

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2819.38859374 Predicted Change= -3.799676D-08
Zero-point correction (ZPE)= -2819.3095 0.07900
Internal Energy (U)= -2819.3040 0.08458
Enthalpy (H)= -2819.3030 0.08552
Gibbs Free Energy (G)= -2819.3404 0.04817

Frequencies -- 174.8006 248.1191 318.8286

Supporting Information: **4bromo2radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3BrN(2) C1[X(C5H3BrN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -2818.71019547 Predicted Change= -8.596147D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00075	0.00180	[YES]	0.00075	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.159970	0.369071	-0.000004
C	0.007828	-0.411933	0.000002
C	-1.178223	0.320606	0.000000
C	-1.156771	1.720580	0.000003
C	0.080199	2.357417	0.000006
N	1.232424	1.654314	-0.000003
H	0.020032	-1.495017	0.000001
H	-2.077342	2.292039	0.000002
H	0.156749	3.441788	0.000001
Br	-2.857439	-0.590965	0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2818.71019547 Predicted Change= -8.596147D-08
Zero-point correction (ZPE)= -2818.6441 0.06605
Internal Energy (U)= -2818.6385 0.07162
Enthalpy (H)= -2818.6376 0.07256
Gibbs Free Energy (G)= -2818.6755 0.03462

Frequencies -- 170.7741 255.3885 308.9726

Supporting Information: **4bromopyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H4BrN C1[X(C5H4BrN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -2819.38918253 Predicted Change= -4.482856D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00037	0.00180	[YES]	0.00037	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.197911	-1.140277	0.000002
C	0.802768	-1.204239	0.000003
C	0.105176	0.000003	0.000019
C	0.802769	1.204240	0.000009
C	2.197914	1.140274	-0.000014
N	2.898266	-0.000001	-0.000004
H	2.778328	-2.061349	-0.000011
H	0.285457	-2.157039	0.000002
H	0.285465	2.157045	0.000021
H	2.778330	2.061347	0.000003
Br	-1.801562	0.000000	-0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2819.38918253 Predicted Change= -4.482856D-08
Zero-point correction (ZPE)= -2819.3101 0.07898
Internal Energy (U)= -2819.3046 0.08455
Enthalpy (H)= -2819.3036 0.08549
Gibbs Free Energy (G)= -2819.3410 0.04815

Frequencies -- 172.5261 253.7692 312.8977

Supporting Information: **5bromo2radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C5H3BrN(2) C1[X(C5H3BrN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -2818.70824815 Predicted Change= -1.145992D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00047	0.00180	[YES]	0.00047	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.320483	0.003057	-0.000187
C	-0.714687	1.257530	-0.000114
C	0.681385	1.254268	0.000074
C	1.352672	0.025946	0.000185
C	0.631982	-1.164597	0.000110
N	-0.715282	-1.134013	-0.000087
H	1.243407	2.183306	0.000136
H	-1.280416	2.182934	-0.000209
H	1.123845	-2.132619	0.000182
Br	3.259693	-0.025873	0.000444

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2818.70824815 Predicted Change= -1.145992D-07
Zero-point correction (ZPE)= -2818.6421 0.06607
Internal Energy (U)= -2818.6366 0.07164
Enthalpy (H)= -2818.6356 0.07258
Gibbs Free Energy (G)= -2818.6735 0.03465

Frequencies -- 186.2288 250.1214 320.2949

Bromopyrimidines

Supporting Information: **24dibromopyrimidine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Br2N2 C1[X(C4H2Br2N2)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -5406.53025356 Predicted Change= -1.356932D-06

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00044	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00125	0.00180	[YES]	0.00125	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.121802	0.367320	0.000158
N	-0.001086	-0.351390	0.000073
C	1.120536	0.348859	0.000026
C	1.155257	1.743275	0.000034
C	-0.089210	2.366310	0.000033
N	-1.245434	1.687471	0.000071
H	2.084103	2.298877	0.000018
H	-0.169237	3.451265	0.000015
Br	-2.744999	-0.629792	-0.000090
Br	2.757058	-0.628988	0.000017

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5406.53025356 Predicted Change= -1.356932D-06

Zero-point correction (ZPE)= -5406.4738 0.05640

Internal Energy (U)= -5406.4669 0.06328

Enthalpy (H)= -5406.4660 0.06422

Gibbs Free Energy (G)= -5406.5079 0.02233

Frequencies -- 136.1364 147.8878 158.9081

Supporting Information: **25dibromopyrimidine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Br2N2 C1[X(C4H2Br2N2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -5406.52707357 Predicted Change= -5.140991D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00039	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00058	0.00180	[YES]	0.00058	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.309126	0.000000	0.000048
N	-0.727269	1.194373	0.000025
C	0.609838	1.190402	0.000008
C	1.335057	0.000000	0.000004
C	0.609837	-1.190402	0.000006
N	-0.727270	-1.194373	0.000022
H	1.107346	2.156972	0.000004
H	1.107345	-2.156971	-0.000001
Br	-3.215979	0.000000	-0.000009
Br	3.230077	0.000000	-0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5406.52707357 Predicted Change= -5.140991D-07
Zero-point correction (ZPE)= -5406.4705 0.05652
Internal Energy (U)= -5406.4636 0.06344
Enthalpy (H)= -5406.4626 0.06439
Gibbs Free Energy (G)= -5406.5046 0.02241

Frequencies -- 67.9986 164.5648 221.7971

Supporting Information: **2bromo4radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrN2(2) C1[X(C4H2BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -2834.74758033 Predicted Change= -2.764088D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00029	0.00180	[YES]	0.00029	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.137691	0.362651	-0.000014
N	0.008949	-0.335432	0.000034
C	1.099971	0.354890	0.000055
C	1.169125	1.743298	0.000049
C	-0.083179	2.362485	0.000039
N	-1.238967	1.679397	0.000013
H	2.095477	2.305053	0.000063
H	-0.171128	3.447830	0.000041
Br	-2.754430	-0.637976	0.000058

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2834.74758033 Predicted Change= -2.764088D-08
Zero-point correction (ZPE)= -2834.6937 0.05381
Internal Energy (U)= -2834.6883 0.05925
Enthalpy (H)= -2834.6873 0.06019
Gibbs Free Energy (G)= -2834.7251 0.02245

Frequencies -- 147.8870 273.9726 327.7314

Supporting Information: **2bromo5radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq ub3lyp/6-31g(d) nosymm geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrN2(2) C1[X(C4H2BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -2834.73484468 Predicted Change= -2.930173D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00113	0.00180	[YES]	0.00113	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.300731	0.000000	-0.000118
N	-0.727453	1.198382	-0.000025
C	0.620599	1.200079	0.000029
C	1.297928	0.000000	0.000031
C	0.620598	-1.200079	0.000025
N	-0.727453	-1.198381	-0.000028
H	1.109441	2.170772	0.000037
H	1.109440	-2.170772	0.000033
Br	-3.212590	0.000000	0.000123

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2834.73484468 Predicted Change= -2.930173D-07
Zero-point correction (ZPE)= -2834.6810 0.05381
Internal Energy (U)= -2834.6755 0.05927
Enthalpy (H)= -2834.6746 0.06021
Gibbs Free Energy (G)= -2834.7124 0.02243

Frequencies -- 161.2169 268.7679 324.5271

Supporting Information: **2bromopyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN2 C1[X(C4H3BrN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2835.42639139 Predicted Change= -2.074626D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00088	0.00180	[YES]	0.00088	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.149969	-0.000002	-0.000023
N	0.726901	-1.195768	-0.000009
C	2.066335	-1.183106	0.000003
C	2.802304	0.000001	0.000007
C	2.066332	1.183107	0.000003
N	0.726899	1.195767	-0.000006
H	2.552760	-2.156660	0.000003
H	3.886668	0.000002	0.000013
H	2.552757	2.156661	0.000009
Br	-1.762241	0.000000	0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2835.42639139 Predicted Change= -2.074626D-07
Zero-point correction (ZPE)= -2835.3596 0.06675
Internal Energy (U)= -2835.3541 0.07223
Enthalpy (H)= -2835.3532 0.07318
Gibbs Free Energy (G)= -2835.3904 0.03595

Frequencies -- 146.1922 272.5902 322.4937

Supporting Information: **2bromopyrimidineradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -263.642061272 Predicted Change= -6.675453D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00035	0.00180	[YES]	0.00035	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.000000	-1.326550	-0.000011
N	1.193074	-0.785395	-0.000008
C	1.190742	0.561822	0.000003
C	0.000000	1.288489	0.000011
C	-1.190741	0.561822	0.000006
N	-1.193074	-0.785394	-0.000005
H	2.161263	1.054365	0.000007
H	0.000001	2.373295	0.000021
H	-2.161263	1.054366	0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -263.642061272 Predicted Change= -6.675453D-08
Zero-point correction (ZPE)= -263.5779 0.06407
Internal Energy (U)= -263.5738 0.06825
Enthalpy (H)= -263.5728 0.06919
Gibbs Free Energy (G)= -263.6059 0.03614

Frequencies -- 379.6524 383.2477 586.1641

Supporting Information: **4bromo2radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrN2(2) C1[X(C4H2BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -2834.74635122 Predicted Change= -3.211446D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00024	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00077	0.00180	[YES]	0.00077	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.095523	0.384054	0.000102
N	-0.010313	-0.357109	0.000092
C	1.122199	0.340354	0.000066
C	1.145497	1.737831	0.000028
C	-0.093281	2.374353	0.000047
N	-1.250549	1.680289	0.000086
H	2.075834	2.291496	-0.000011
H	-0.167820	3.459715	0.000024
Br	2.764140	-0.627983	0.000011

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2834.74635122 Predicted Change= -3.211446D-07
Zero-point correction (ZPE)= -2834.6924 0.05389
Internal Energy (U)= -2834.6870 0.05933
Enthalpy (H)= -2834.6860 0.06027
Gibbs Free Energy (G)= -2834.7238 0.02250

Frequencies -- 157.4607 266.3327 312.6770

Supporting Information: **4bromopyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN2 C1[X(C4H3BrN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2835.42897171 Predicted Change= -3.996250D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00056	0.00180	[YES]	0.00056	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.078913	-1.150670	0.000015
N	-0.738035	-1.184766	0.000004
C	-0.134896	-0.010931	0.000008
C	-0.817244	1.205447	0.000007
C	-2.206035	1.108031	0.000008
N	-2.854106	-0.065606	0.000013
H	-2.581036	-2.115291	0.000005
H	-0.301076	2.157654	0.000006
H	-2.822517	2.005119	0.000014
Br	1.779204	-0.005890	-0.000011

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2835.42897171 Predicted Change= -3.996250D-07
Zero-point correction (ZPE)= -2835.3619 0.06703
Internal Energy (U)= -2835.3564 0.07251
Enthalpy (H)= -2835.3555 0.07345
Gibbs Free Energy (G)= -2835.3927 0.03623

Frequencies -- 157.7627 264.0413 309.2432

Supporting Information: **4bromopyrimidineradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -263.646149248 Predicted Change= -2.527220D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00053	0.00180	[YES]	0.00053	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.244944	0.378620	-0.000042
N	1.030948	-0.954898	0.000010
C	-0.196020	-1.354071	0.000017
C	-1.303840	-0.513461	0.000002
C	-0.978361	0.845762	0.000011
N	0.285392	1.297614	-0.000006
H	2.276944	0.719847	0.000030
H	-2.330079	-0.863083	0.000001
H	-1.761583	1.603124	0.000006

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -263.646149248 Predicted Change= -2.527220D-07
Zero-point correction (ZPE)= -263.5818 0.06427
Internal Energy (U)= -263.5777 0.06843
Enthalpy (H)= -263.5767 0.06937
Gibbs Free Energy (G)= -263.6097 0.03635

Frequencies -- 349.6043 435.7294 602.1459

Supporting Information: **5bromo2radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrN2(2) C1[X(C4H2BrN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -2834.74259275 Predicted Change= -2.214107D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00045	0.00180	[YES]	0.00045	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.280272	0.000000	0.000033
N	-0.736542	1.191014	0.000028
C	0.608420	1.197855	0.000013
C	1.324784	0.000000	0.000003
C	0.608419	-1.197855	0.000011
N	-0.736542	-1.191013	0.000026
H	1.111421	2.161583	0.000007
H	1.111420	-2.161583	0.000002
Br	3.224726	0.000000	-0.000020

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2834.74259275 Predicted Change= -2.214107D-07
Zero-point correction (ZPE)= -2834.6885 0.05402
Internal Energy (U)= -2834.6830 0.05949
Enthalpy (H)= -2834.6821 0.06044
Gibbs Free Energy (G)= -2834.7199 0.02262

Frequencies -- 185.9838 245.2056 324.9357

Supporting Information: **5bromopyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN2 C1[X(C4H3BrN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2835.42591474 Predicted Change= -5.986460D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.771380	-0.000001	0.000005
N	2.175511	-1.197010	0.000002
C	0.838957	-1.192570	0.000000
C	0.117467	0.000000	-0.000002
C	0.838958	1.192571	-0.000004
N	2.175512	1.197010	0.000000
H	0.333414	-2.155708	0.000002
H	3.858986	0.000000	0.000003
H	0.333415	2.155709	-0.000002
Br	-1.782387	0.000000	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2835.42591474 Predicted Change= -5.986460D-08
Zero-point correction (ZPE)= -2835.3587 0.06719
Internal Energy (U)= -2835.3532 0.07268
Enthalpy (H)= -2835.3522 0.07362
Gibbs Free Energy (G)= -2835.3895 0.03638

Frequencies -- 172.9330 243.9467 322.9716

Supporting Information: **5bromopyrimidineradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -263.634206758 Predicted Change= -1.719951D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00089	0.00180	[YES]	0.00089	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	1.240533	0.000005
N	-1.200971	0.653718	-0.000002
C	-1.201978	-0.694199	-0.000002
C	0.000000	-1.368860	0.000002
C	1.201978	-0.694199	-0.000003
N	1.200972	0.653718	0.000000
H	-2.169723	-1.190249	0.000001
H	0.000000	2.328795	-0.000007
H	2.169723	-1.190250	0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -263.634206758 Predicted Change= -1.719951D-07
Zero-point correction (ZPE)= -263.5699 0.06430
Internal Energy (U)= -263.5657 0.06846
Enthalpy (H)= -263.5648 0.06940
Gibbs Free Energy (G)= -263.5978 0.03637

Frequencies -- 381.5943 399.0817 567.7578

Bromopyrroles

Supporting Information: **23dibromopyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3Br2N C1[X(C4H3Br2N)] #Atoms= 10

Charge = 0 Multiplicity = 1

SCF Energy= -5352.36898278 Predicted Change= -3.408782D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00047	0.00180	[YES]	0.00047	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.122636	2.778893	0.000151
C	-1.053974	2.063458	0.000100
C	-0.701951	0.685738	0.000094
C	0.672676	0.605224	-0.000030
N	1.168230	1.884428	-0.000010
H	2.150877	2.112334	-0.000099
H	0.302369	3.843767	0.000224
H	-2.056349	2.465785	0.000146
Br	1.797955	-0.888414	-0.000186
Br	-1.878264	-0.780522	0.000126

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5352.36898278 Predicted Change= -3.408782D-08

Zero-point correction (ZPE)= -5352.3060 0.06292

Internal Energy (U)= -5352.2993 0.06958

Enthalpy (H)= -5352.2984 0.07053

Gibbs Free Energy (G)= -5352.3394 0.02955

Frequencies -- 103.2135 179.4841 227.5407

Supporting Information: **2bromopyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4BrN C1[X(C4H4BrN)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2781.26768188 Predicted Change= -3.657514D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00060	0.00180	[YES]	0.00060	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.415638	-0.714662	0.000228
C	2.499751	0.660342	0.000164
C	1.171919	1.179948	0.000189
C	0.329521	0.093057	0.000030
N	1.080909	-1.053994	0.000128
H	0.699736	-1.987545	0.000014
H	3.181017	-1.476752	0.000305
H	3.413604	1.238689	0.000199
H	0.868128	2.216511	0.000227
Br	-1.549423	0.002141	-0.000152

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2781.26768188 Predicted Change= -3.657514D-08
Zero-point correction (ZPE)= -2781.1948 0.07280
Internal Energy (U)= -2781.1896 0.07807
Enthalpy (H)= -2781.1886 0.07902
Gibbs Free Energy (G)= -2781.2249 0.04277

Frequencies -- 198.7158 252.8478 362.1089

Supporting Information: **2radical3bromopyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN(2) C1[X(C4H3BrN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -2780.56671497 Predicted Change= -1.287646D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00087	0.00180	[YES]	0.00087	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.123625	2.781847	-0.000154
C	-1.048841	2.060600	0.000383
C	-0.701705	0.671644	-0.000086
C	0.664211	0.623808	-0.000036
N	1.178553	1.882758	0.000185
H	2.159018	2.117745	0.000222
H	0.301199	3.847624	-0.000328
H	-2.053825	2.458961	0.000656
Br	-1.895984	-0.785883	-0.000140

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2780.56671497 Predicted Change= -1.287646D-07
Zero-point correction (ZPE)= -2780.5076 0.05908
Internal Energy (U)= -2780.5026 0.06402
Enthalpy (H)= -2780.5017 0.06496
Gibbs Free Energy (G)= -2780.5380 0.02868

Frequencies -- -74.3784 247.4541 301.4714

Supporting Information: **3bromopyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4BrN C1[X(C4H4BrN)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -2781.26875010 Predicted Change= -5.139210D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00024	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00188	0.00180	[NO]	0.00188	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.441918	0.711637	0.000067
C	1.140568	1.165433	0.000119
C	0.312354	0.010607	-0.000002
C	1.113373	-1.108686	-0.000022
N	2.413476	-0.662830	0.000007
H	3.225439	-1.260842	-0.000133
H	3.377224	1.252219	0.000114
H	0.812148	2.194386	0.000203
H	0.861895	-2.157885	-0.000078
Br	-1.577723	-0.001772	-0.000032

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2781.26875010 Predicted Change= -5.139210D-07
Zero-point correction (ZPE)= -2781.1958 0.07293
Internal Energy (U)= -2781.1905 0.07819
Enthalpy (H)= -2781.1896 0.07913
Gibbs Free Energy (G)= -2781.2258 0.04293

Frequencies -- 219.6058 249.9147 356.6598

Supporting Information: **3bromopyrroleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4N(2) C1[X(C4H4N)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -209.467949548 Predicted Change= -1.832441D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00117	0.00180	[YES]	0.00117	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.436334	0.709598	0.000089
C	1.131273	1.173565	0.000100
C	0.329286	0.011554	0.000066
C	1.103402	-1.117382	-0.000036
N	2.412071	-0.664931	-0.000016
H	3.230355	-1.255415	-0.000130
H	3.373645	1.248749	0.000129
H	0.818361	2.207841	0.000168
H	0.863666	-2.169539	-0.000096

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -209.467949548 Predicted Change= -1.832441D-07
Zero-point correction (ZPE)= -209.3981 0.06976
Internal Energy (U)= -209.3941 0.07380
Enthalpy (H)= -209.3931 0.07475
Gibbs Free Energy (G)= -209.4252 0.04274

Frequencies -- 406.2465 537.5173 633.4816

Supporting Information: **2bromopyrroleradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H4N(2) C1[X(C4H4N)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -209.466819346 Predicted Change= -3.209980D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00145	0.00180	[YES]	0.00145	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.417127	-0.717278	0.000034
C	2.496588	0.657247	0.000369
C	1.162684	1.190137	0.000035
C	0.347058	0.091119	0.000077
N	1.072988	-1.059605	0.000251
H	0.698986	-1.995449	0.000234
H	3.184935	-1.477621	-0.000067
H	3.410391	1.237686	0.000556
H	0.869466	2.229359	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -209.466819346 Predicted Change= -3.209980D-07
Zero-point correction (ZPE)= -209.3976 0.06921
Internal Energy (U)= -209.3933 0.07345
Enthalpy (H)= -209.3924 0.07440
Gibbs Free Energy (G)= -209.4248 0.04199

Frequencies -- 272.2314 444.0314 618.1534

Supporting Information: **3radical2bromopyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrN(2) C1[X(C4H3BrN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -2780.56771952 Predicted Change= -1.077140D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00093	0.00180	[YES]	0.00093	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.120704	2.773540	0.000362
C	-1.067334	2.062611	-0.000010
C	-0.689835	0.702061	0.000113
C	0.670573	0.594083	0.000062
N	1.168812	1.881084	-0.000222
H	2.150679	2.115711	-0.000461
H	0.302064	3.839163	0.000580
H	-2.064306	2.479037	-0.000037
Br	1.811112	-0.896078	0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2780.56771952 Predicted Change= -1.077140D-07
Zero-point correction (ZPE)= -2780.5077 0.05994
Internal Energy (U)= -2780.5024 0.06527
Enthalpy (H)= -2780.5015 0.06621
Gibbs Free Energy (G)= -2780.5384 0.02922

Frequencies -- 179.1985 251.4565 366.5613

Bromoxazoles

Supporting Information: **2bromooxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNO C1[X(C3H2BrNO)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -2817.16671029 Predicted Change= -2.552798D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00160	0.00180	[YES]	0.00160	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.351421	-0.684918	0.000162
C	2.387383	0.669214	0.000193
C	0.355671	0.105043	0.000062
H	3.080610	-1.478746	0.000223
H	3.241819	1.330297	0.000264
N	1.086349	1.168767	-0.000049
O	1.029859	-1.069500	0.000094
Br	-1.506646	-0.000370	-0.000097

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2817.16671029 Predicted Change= -2.552798D-07

Zero-point correction (ZPE)= -2817.1181 0.04855

Internal Energy (U)= -2817.1133 0.05332

Enthalpy (H)= -2817.1124 0.05427

Gibbs Free Energy (G)= -2817.1478 0.01885

Frequencies -- 216.2019 274.1142 373.9288

Supporting Information: **5bromooxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNO C1[X(C3H2BrNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -2817.16727767 Predicted Change= -8.121831D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00048	0.00180	[YES]	0.00048	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.334918	0.104663	0.000022
C	1.206930	1.144402	0.000049
C	2.343312	-0.647084	0.000185
H	0.998092	2.203529	0.000005
H	3.095427	-1.422194	0.000239
N	2.500676	0.637192	0.000114
O	1.046035	-1.062377	0.000079
Br	-1.522214	-0.010130	-0.000092

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2817.16727767 Predicted Change= -8.121831D-08
Zero-point correction (ZPE)= -2817.1184 0.04882
Internal Energy (U)= -2817.1136 0.05359
Enthalpy (H)= -2817.1127 0.05454
Gibbs Free Energy (G)= -2817.1481 0.01907

Frequencies -- 216.4021 258.6710 369.0466

Supporting Information: **4bromooxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C3H2BrNO C1[X(C3H2BrNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -2817.16917476 Predicted Change= -2.432846D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.144688	1.100608	0.000003
C	-0.333598	0.012928	0.000011
C	-2.307403	-0.712882	0.000126
H	-0.994720	2.167032	-0.000057
H	-3.220538	-1.289566	0.000177
N	-1.085922	-1.144765	0.000141
O	-2.434635	0.637477	0.000055
Br	1.543084	-0.010510	-0.000068

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2817.16917476 Predicted Change= -2.432846D-07
Zero-point correction (ZPE)= -2817.1203 0.04880
Internal Energy (U)= -2817.1156 0.05356
Enthalpy (H)= -2817.1146 0.05451
Gibbs Free Energy (G)= -2817.1500 0.01908

Frequencies -- 234.8194 266.1350 362.3112

Bromothiophenes

Supporting Information: **23dibromothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Br2S C1[X(C4H2Br2S)] #Atoms= 9

Charge = 0 Multiplicity = 1

SCF Energy= -5695.20269054 Predicted Change= -9.595885D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.800189	2.682038	0.000113
C	-0.476755	2.201685	-0.000027
C	-0.518961	0.773112	0.000000
C	0.723028	0.199307	0.000009
S	1.978712	1.404405	-0.000136
H	1.124660	3.713929	0.000207
H	-1.365518	2.820590	-0.000027
Br	1.145094	-1.626730	0.000032
Br	-2.133195	-0.205894	0.000009

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5695.20269054 Predicted Change= -9.595885D-08

Zero-point correction (ZPE)= -5695.1556 0.04704

Internal Energy (U)= -5695.1487 0.05391

Enthalpy (H)= -5695.1478 0.05486

Gibbs Free Energy (G)= -5695.1896 0.01308

Frequencies -- 111.6414 140.2454 220.0498

Supporting Information: **24dibromothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt freq b3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2Br2S C1[X(C4H2Br2S)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -5695.20288690 Predicted Change= -8.520640D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00068	0.00180	[YES]	0.00068	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.915140	1.547253	0.000068
C	-1.207503	0.215122	0.000010
C	-0.065302	-0.642820	0.000036
C	1.089889	0.084032	-0.000015
S	0.804731	1.801320	-0.000073
H	-1.597862	2.384733	0.000117
H	-0.111583	-1.723702	0.000061
Br	2.848543	-0.586711	-0.000040
Br	-2.979341	-0.461965	0.000052

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -5695.20288690 Predicted Change= -8.520640D-08
Zero-point correction (ZPE)= -5695.1559 0.04698
Internal Energy (U)= -5695.1489 0.05389
Enthalpy (H)= -5695.1480 0.05483
Gibbs Free Energy (G)= -5695.1900 0.01287

Frequencies -- 127.6533 133.6650 227.7545

Supporting Information: **2bromo3radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrS(2) C1[X(C4H2BrS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -3123.40750004 Predicted Change= -2.693128D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00113	0.00180	[YES]	0.00113	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.794448	2.684938	-0.000132
C	-0.489807	2.206254	0.000159
C	-0.481160	0.789322	0.000029
C	0.720727	0.182802	-0.000165
S	1.983032	1.410335	0.000648
H	1.122041	3.716927	-0.000287
H	-1.377171	2.827498	0.000163
Br	1.138339	-1.649739	-0.000244

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3123.40750004 Predicted Change= -2.693128D-07
Zero-point correction (ZPE)= -3123.3631 0.04433
Internal Energy (U)= -3123.3577 0.04979
Enthalpy (H)= -3123.3567 0.05073
Gibbs Free Energy (G)= -3123.3946 0.01287

Frequencies -- 171.9308 205.4429 330.8212

Supporting Information: **2bromo4radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrS(2) C1[X(C4H2BrS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -3123.40992178 Predicted Change= -3.105524D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ‖	0.00045	[YES]	0.00000 ‖	0.00030	[YES]
Displ	0.00009 ‖	0.00180	[YES]	0.00009 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.936904	1.553293	0.000043
C	-1.175447	0.228083	0.000071
C	-0.069900	-0.657736	0.000035
C	1.085928	0.078001	-0.000014
S	0.809172	1.799985	-0.000013
H	-1.607948	2.400444	0.000064
H	-0.111084	-1.739011	0.000047
Br	2.851956	-0.583832	-0.000070

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3123.40992178 Predicted Change= -3.105524D-09
Zero-point correction (ZPE)= -3123.3657 0.04418
Internal Energy (U)= -3123.3602 0.04965
Enthalpy (H)= -3123.3593 0.05059
Gibbs Free Energy (G)= -3123.3971 0.01278

Frequencies -- 186.4028 212.4842 329.9215

Supporting Information: **2bromothiophene.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrS C1[X(C4H3BrS)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -3124.10129651 Predicted Change= -2.992047D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00041	0.00180	[YES]	0.00041	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.584370	-0.203715	0.000029
C	-2.266759	1.125558	-0.000090
C	-0.857453	1.367157	0.000089
C	-0.142089	0.203302	0.000001
S	-1.163440	-1.205444	0.000005
H	-3.564728	-0.661059	0.000042
H	-3.008703	1.916669	-0.000150
H	-0.398939	2.348688	0.000135
Br	1.734041	0.020828	-0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3124.10129651 Predicted Change= -2.992047D-08
Zero-point correction (ZPE)= -3124.0442 0.05702
Internal Energy (U)= -3124.0388 0.06245
Enthalpy (H)= -3124.0378 0.06340
Gibbs Free Energy (G)= -3124.0750 0.02626

Frequencies -- 189.0153 212.7394 330.8773

Supporting Information: **2bromothiopheneradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3S(2) C1[X(C4H3S)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -552.306314949 Predicted Change= -4.897337D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00173	0.00180	[YES]	0.00173	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.584552	-0.205046	-0.000138
C	-2.264711	1.123804	0.000107
C	-0.845110	1.375366	-0.000016
C	-0.173271	0.198976	-0.000011
S	-1.152592	-1.214684	0.000309
H	-3.565497	-0.661941	-0.000255
H	-3.008131	1.914748	0.000139
H	-0.392617	2.359933	-0.000073

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -552.306314949 Predicted Change= -4.897337D-07
Zero-point correction (ZPE)= -552.2522 0.05408
Internal Energy (U)= -552.2480 0.05822
Enthalpy (H)= -552.2471 0.05916
Gibbs Free Energy (G)= -552.2801 0.02618

Frequencies -- 364.1643 515.5377 605.8005

Supporting Information: **3bromo2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrS(2) C1[X(C4H2BrS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -3123.40614137 Predicted Change= -1.279553D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008 ‖	0.00045	[YES]	0.00003 ‖	0.00030	[YES]
Displ	0.00090 ‖	0.00180	[YES]	0.00090 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.801610	2.681990	-0.000215
C	-0.476702	2.203158	0.000307
C	-0.526426	0.765300	-0.000052
C	0.717400	0.236199	-0.000183
S	1.988686	1.391238	0.000475
H	1.131466	3.712680	-0.000366
H	-1.364602	2.824932	0.000481
Br	-2.139270	-0.226325	-0.000300

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3123.40614137 Predicted Change= -1.279553D-07
Zero-point correction (ZPE)= -3123.3618 0.04428
Internal Energy (U)= -3123.3563 0.04978
Enthalpy (H)= -3123.3554 0.05073
Gibbs Free Energy (G)= -3123.3934 0.01273

Frequencies -- 151.7125 227.9923 319.0283

Supporting Information: **3bromothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt=(modredundant) freq b3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3BrS C1[X(C4H3BrS)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -3124.10509619 Predicted Change= -4.467659D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00052	0.00180	[YES]	0.00052	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.073358	1.122617	-0.000104
C	0.719879	1.303223	0.000159
C	0.022277	0.057037	-0.000032
C	0.834843	-1.039299	0.000098
S	2.502400	-0.559839	-0.000017
H	2.846927	1.878573	-0.000196
H	0.226849	2.267536	0.000250
H	0.554677	-2.082534	0.000151
Br	-1.873400	-0.050503	-0.000019

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3124.10509619 Predicted Change= -4.467659D-08
Zero-point correction (ZPE)= -3124.0480 0.05705
Internal Energy (U)= -3124.0426 0.06245
Enthalpy (H)= -3124.0416 0.06340
Gibbs Free Energy (G)= -3124.0787 0.02632

Frequencies -- 190.8755 239.6278 318.7750

Supporting Information: **3bromothiopheneradical.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d) geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H3S(2) C1[X(C4H3S)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -552.310852239 Predicted Change= -3.327602D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00145	0.00180	[YES]	0.00145	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.069889	1.126617	0.000167
C	0.711755	1.313345	-0.000088
C	0.053335	0.057790	0.000079
C	0.816580	-1.053287	0.000314
S	2.505321	-0.557419	-0.000864
H	2.847348	1.879952	0.000323
H	0.225001	2.281138	-0.000038
H	0.551980	-2.100822	0.000415

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -552.310852239 Predicted Change= -3.327602D-07
Zero-point correction (ZPE)= -552.2567 0.05410
Internal Energy (U)= -552.2526 0.05819
Enthalpy (H)= -552.2517 0.05913
Gibbs Free Energy (G)= -552.2845 0.02625

Frequencies -- 435.0858 548.3101 598.5436

Supporting Information: **4bromo2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

opt nosymm freq ub3lyp/6-31g(d)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C4H2BrS(2) C1[X(C4H2BrS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -3123.40894829 Predicted Change= -5.191900D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00212	0.00180	[NO]	0.00212	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.914723	1.548105	-0.000022
C	-1.203732	0.214831	0.000093
C	-0.057019	-0.657602	-0.000003
C	1.061139	0.103563	-0.000044
S	0.818223	1.804836	0.000128
H	-1.598921	2.384964	-0.000039
H	-0.107729	-1.738466	-0.000035
Br	-2.979350	-0.456258	0.000178

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3123.40894829 Predicted Change= -5.191900D-07
Zero-point correction (ZPE)= -3123.3646 0.04426
Internal Energy (U)= -3123.3592 0.04972
Enthalpy (H)= -3123.3582 0.05066
Gibbs Free Energy (G)= -3123.3961 0.01284

Frequencies -- 184.1267 240.0294 316.0657

Molecular Geometries: *G3B3*

Chlorooxatriazoles

Supporting Information: **4chloro1235oxatriazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= CClN3O C1[X(CClN3O)] #Atoms= 6
Charge = 0 Multiplicity = 1

SCF Energy= -735.533664014 Predicted Change= -8.973158D-07
MP2 Energy= -737.2390026327 Correl. Energy= -1.70533861

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00042	0.00045	[YES]	0.00014	0.00030	[YES]
Displ	0.00100	0.00180	[YES]	0.00100	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.217092	-0.026018	-0.000404
O	1.774732	-0.658651	-0.000218
N	1.760174	0.747653	-0.000026
N	0.558459	1.117735	0.000396
N	0.498633	-1.117421	0.000448
Cl	-1.918598	0.011149	-0.000092

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -735.533664014 Predicted Change= -8.973158D-07
MP2 Energy= -737.2390026327 MP2 Cor. Energy= -1.70533861
Zero-point correction (ZPE)= -737.6376 0.02386
Internal Energy (U)= -737.6333 0.02824
Enthalpy (H)= -737.6323 0.02919
Gibbs Free Energy (G)= -737.6661 -0.00461

Frequencies -- 268.8013 327.1403 512.3390

Supporting Information: **4radical1235oxatriazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=(restart,maxcycle=10000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= CN3O(2) C1[X(CN3O)] #Atoms= 5
Charge = 0 Multiplicity = 2

SCF Energy= -275.957784686 Predicted Change= -5.339650D-07
MP2 Energy= -277.0716633722 Correl. Energy= -1.11387868

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00015	0.00030	[YES]
Displ	0.00087	0.00180	[YES]	0.00087	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.162179	1.112467	0.000112
O	0.540548	-0.924534	-0.000092
N	-0.853189	-0.724599	0.000224
N	-1.069737	0.521895	-0.000243
N	1.166146	0.305772	0.000029

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -275.957784686 Predicted Change= -5.339650D-07
MP2 Energy= -277.0716633722 MP2 Cor. Energy= -1.11387868
Zero-point correction (ZPE)= -277.3510 0.02010
Internal Energy (U)= -277.3476 0.02351
Enthalpy (H)= -277.3466 0.02445
Gibbs Free Energy (G)= -277.3776 -0.00655

Frequencies -- 619.1436 639.8158 684.9325

Chlorotriazines

Supporting Information: **4chloro123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -737.622763334 Predicted Change= -4.307017D-07
MP2 Energy= -739.4310502797 Correl. Energy= -1.80828694

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00115	0.00180	[YES]	0.00115	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.148023	-1.174295	0.000025
C	0.455038	0.009832	0.000010
C	-0.240940	1.213303	-0.000012
C	-1.618484	1.066970	-0.000019
N	-2.217376	-0.135330	0.000038
H	0.253494	2.177863	-0.000004
H	-2.287159	1.923753	0.000018
N	-1.479651	-1.230846	-0.000010
Cl	2.198549	-0.003468	-0.000015

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.622763334 Predicted Change= -4.307017D-07
MP2 Energy= -739.4310502797 MP2 Cor. Energy= -1.80828694
Zero-point correction (ZPE)= -739.8371 0.05381
Internal Energy (U)= -739.8318 0.05910
Enthalpy (H)= -739.8309 0.06004

Supporting Information: **4radical123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -278.044319477 Predicted Change= -1.621169D-07
MP2 Energy= -279.3260907571 Correl. Energy= -1.28177128

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00055	0.00180	[YES]	0.00055	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.076999	-0.883127	-0.000015
C	-0.120561	-1.340327	0.000001
C	-1.274863	-0.564670	0.000021
C	-0.998661	0.793941	0.000018
N	0.264108	1.272523	-0.000021
H	-2.284007	-0.962580	0.000004
H	-1.782347	1.548040	-0.000009
N	1.291873	0.479300	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -278.044319477 Predicted Change= -1.621169D-07
MP2 Energy= -279.3260907571 MP2 Cor. Energy= -1.28177128
Zero-point correction (ZPE)= -279.5674 0.05003
Internal Energy (U)= -279.5631 0.05432
Enthalpy (H)= -279.5622 0.05526
Gibbs Free Energy (G)= -279.5954 0.02200

Supporting Information: **5chloro123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -737.620271883 Predicted Change= -2.709460D-07
MP2 Energy= -739.4287868258 Correl. Energy= -1.80851494

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.593987	-1.154438	0.000006
C	-0.255087	-1.176003	-0.000001
C	0.482987	-0.000001	-0.000004
C	-0.255089	1.176004	-0.000003
N	-1.593985	1.154441	0.000010
H	0.213170	-2.156507	-0.000006
H	0.213172	2.156506	0.000000
N	-2.245496	-0.000002	0.000004
Cl	2.221827	0.000000	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.620271883 Predicted Change= -2.709460D-07
MP2 Energy= -739.4287868258 MP2 Cor. Energy= -1.80851494
Zero-point correction (ZPE)= -739.8351 0.05393
Internal Energy (U)= -739.8298 0.05925
Enthalpy (H)= -739.8288 0.06019

Supporting Information: **5radical123triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -278.038953595 Predicted Change= -3.181334D-08
MP2 Energy= -279.314530077 Correl. Energy= -1.27557648

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00040 ‖	0.00180	[YES]	0.00040 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.150240	-0.680360	-0.000002
C	-1.179842	0.678881	0.000003
C	-0.000001	1.377018	0.000006
C	1.179840	0.678882	0.000005
N	1.150242	-0.680358	-0.000005
H	-2.171480	1.121196	0.000007
H	2.171478	1.121200	0.000000
N	0.000001	-1.303723	-0.000007

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -278.038953595 Predicted Change= -3.181334D-08
MP2 Energy= -279.314530077 MP2 Cor. Energy= -1.27557648
Zero-point correction (ZPE)= -279.5618 0.05051
Internal Energy (U)= -279.5576 0.05469
Enthalpy (H)= -279.5567 0.05563
Gibbs Free Energy (G)= -279.5897 0.02257

Supporting Information: **3chloro124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -737.652537804 Predicted Change= -6.461034D-07
MP2 Energy= -739.4559608155 Correl. Energy= -1.80342301

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00106	0.00180	[YES]	0.00106	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	0.140906	-1.192192	0.000086
C	-0.432775	0.012658	0.000224
C	1.490888	1.148428	0.000008
C	2.151469	-0.083995	-0.000006
N	1.475133	-1.233423	0.000010
H	2.030694	2.093254	-0.000006
H	3.234233	-0.164188	-0.000039
N	0.162492	1.204874	0.000088
Cl	-2.174831	0.009034	-0.000153

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.652537804 Predicted Change= -6.461034D-07
MP2 Energy= -739.4559608155 MP2 Cor. Energy= -1.80342301
Zero-point correction (ZPE)= -739.8612 0.05446
Internal Energy (U)= -739.8560 0.05968
Enthalpy (H)= -739.8550 0.06062
Gibbs Free Energy (G)= -739.8909 0.02475

Frequencies -- 150.5448 326.4030 383.6513

Supporting Information: **3radical124triazine.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # g3b3
 #N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
 #N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
 #N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C3H2N3(2)   C1[X(C3H2N3)]  #Atoms= 8
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -278.073319705     Predicted Change= -9.430839D-07
 MP2 Energy= -279.3457139905     Correl. Energy= -1.27239428
=====================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.   Criteria   Pass?     RMS Val.   Criteria   Pass?
 Force      0.00028 ||  0.00045   [ YES ]     0.00012 ||  0.00030   [ YES ]
 Displ      0.00137 ||  0.00180   [ YES ]     0.00137 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic        Coordinates (Angstroms)
      Type      X          Y      Z
---------------------------------------------------------------------
      N       -1.275701     -0.619460     -0.000053
      C       -0.153000     -1.294882     -0.000082
      C        1.228489      0.434692      0.000044
      C        0.079752      1.241131      0.000079
      N       -1.150669      0.732366      0.000032
      H        2.232854      0.853013      0.000064
      H        0.144078      2.325971      0.000141
      N        1.096601     -0.893567     -0.000043
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -278.073319705 Predicted Change= -9.430839D-07
 MP2 Energy=     -279.3457139905        MP2 Cor. Energy= -1.27239428
 Zero-point correction (ZPE)=          -279.5871  0.05088
 Internal Energy (U)=                  -279.5829  0.05506
 Enthalpy (H)=                         -279.5820   0.05600
 Gibbs Free Energy (G)=                -279.6151    0.02292
---------------------------------------------------------------------
 Frequencies --   332.4187              372.3262              567.1038
```

Supporting Information: **5chloro124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -737.655703627 Predicted Change= -3.213738D-07
MP2 Energy= -739.4589245898 Correl. Energy= -1.80322096

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00075	0.00180	[YES]	0.00075	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.233427	0.014811	0.000013
C	1.507092	-1.101042	0.000019
C	-0.456399	-0.035631	-0.000012
C	0.250815	1.178227	0.000000
N	1.579589	1.182984	0.000008
H	2.063343	-2.034402	-0.000007
H	-0.248676	2.141875	0.000002
N	0.164722	-1.191845	-0.000004
Cl	-2.203993	-0.023438	-0.000009

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.655703627 Predicted Change= -3.213738D-07
MP2 Energy= -739.4589245898 MP2 Cor. Energy= -1.80322096
Zero-point correction (ZPE)= -739.8642 0.05474
Internal Energy (U)= -739.8589 0.05996
Enthalpy (H)= -739.8580 0.06091
Gibbs Free Energy (G)= -739.8939 0.02500

Frequencies -- 158.3648 306.3032 379.8374

Supporting Information: **6chloro124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -737.652556113 Predicted Change= -3.574766D-07
MP2 Energy= -739.4562586504 Correl. Energy= -1.80370253

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00035	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00079	0.00180	[YES]	0.00079	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
N	1.495028	-1.213194	-0.000006
C	2.135933	-0.045338	-0.000004
C	0.258404	1.194713	0.000007
C	-0.449049	-0.019674	0.000001
N	0.155174	-1.195471	-0.000005
H	3.220633	-0.103320	0.000009
H	-0.254201	2.153935	0.000010
N	1.581825	1.179427	0.000007
Cl	-2.191903	-0.013185	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.652556113 Predicted Change= -3.574766D-07
MP2 Energy= -739.4562586504 MP2 Cor. Energy= -1.80370253
Zero-point correction (ZPE)= -739.8612 0.05462
Internal Energy (U)= -739.8560 0.05986
Enthalpy (H)= -739.8551 0.06080
Gibbs Free Energy (G)= -739.8910 0.02490

Frequencies -- 164.8113 304.4661 391.9737

Supporting Information: **6radical124triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -278.073109800 Predicted Change= -7.388042D-07
MP2 Energy= -279.3460023944 Correl. Energy= -1.27289259

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00118	0.00180	[YES]	0.00118	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
N	1.366935	0.187103	-0.000001
C	0.438947	1.143949	-0.000036
C	-1.345782	-0.261407	0.000027
C	-0.388803	-1.291095	0.000002
N	0.869811	-1.072369	-0.000004
H	0.818821	2.162426	0.000029
H	-2.418761	-0.430427	0.000005
N	-0.897636	0.988025	0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -278.073109800 Predicted Change= -7.388042D-07
MP2 Energy= -279.3460023944 MP2 Cor. Energy= -1.27289259
Zero-point correction (ZPE)= -279.5891 0.05118
Internal Energy (U)= -279.5850 0.05538
Enthalpy (H)= -279.5840 0.05632
Gibbs Free Energy (G)= -279.6171 0.02323

Frequencies -- 337.0982 378.1195 548.6634

Supporting Information: **2chloro135triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN3 C1[X(C3H2ClN3)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -737.710850586 Predicted Change= -4.736104D-07
MP2 Energy= -739.5002762709 Correl. Energy= -1.78942568

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00076	0.00180	[YES]	0.00076	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.491945	1.119086	0.000009
N	0.156328	1.189102	-0.000004
C	-0.437962	0.000077	-0.000022
C	1.492213	-1.118929	-0.000008
N	2.221755	-0.000166	0.000013
H	2.028608	2.065334	0.000013
H	2.028072	-2.065727	0.000014
N	0.156067	-1.189039	0.000000
Cl	-2.180759	-0.000017	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -737.710850586 Predicted Change= -4.736104D-07
MP2 Energy= -739.5002762709 MP2 Cor. Energy= -1.78942568
Zero-point correction (ZPE)= -739.9051 0.05577
Internal Energy (U)= -739.9000 0.06090
Enthalpy (H)= -739.8990 0.06185
Gibbs Free Energy (G)= -739.9348 0.02611

Frequencies -- 155.0729 333.1210 365.9959

Supporting Information: **2radical135triazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2N3(2) C1[X(C3H2N3)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -278.137269321 Predicted Change= -2.411216D-07
MP2 Energy= -279.3730339892 Correl. Energy= -1.23576466

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00043	0.00180	[YES]	0.00043	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.126402	0.589446	-0.000003
N	-1.184962	-0.755673	-0.000007
C	0.000012	-1.315448	-0.000019
C	1.126378	0.589499	0.000030
N	0.000033	1.305145	0.000014
H	-2.069675	1.131481	0.000012
H	2.069719	1.131417	-0.000009
N	1.184932	-0.755741	-0.000014

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -278.137269321 Predicted Change= -2.411216D-07
MP2 Energy= -279.3730339892 MP2 Cor. Energy= -1.23576466
Zero-point correction (ZPE)= -279.6322 0.05231
Internal Energy (U)= -279.6281 0.05640
Enthalpy (H)= -279.6271 0.05735
Gibbs Free Energy (G)= -279.6601 0.02441

Frequencies -- 326.7783 388.1746 643.2910

Chlorotriazoles

Supporting Information: **4chloro123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3

#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq

#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)

#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)

#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)

#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8

Charge = 0 Multiplicity = 1

SCF Energy= -699.771239885 Predicted Change= -1.333465D-07

MP2 Energy= -701.402708893 Correl. Energy= -1.631469

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00077	0.00180	[YES]	0.00077	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.594780	1.102093	0.000051
C	0.248913	0.012833	-0.000018
N	-1.821740	0.526064	0.000110
H	-2.731218	0.967993	0.000178
H	-0.423623	2.166417	0.000054
N	-1.745961	-0.821011	0.000020
Cl	1.973493	0.010591	-0.000103
N	-0.477918	-1.134197	0.000059

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -699.771239885 Predicted Change= -1.333465D-07

MP2 Energy= -701.402708893 MP2 Cor. Energy= -1.631469

Zero-point correction (ZPE)= -701.7630 0.04969

Internal Energy (U)= -701.7584 0.05430

Enthalpy (H)= -701.7575 0.05525

Gibbs Free Energy (G)= -701.7916 0.02108

Supporting Information: **4radical123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcycle=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -240.188033917 Predicted Change= -1.575899D-08
MP2 Energy= -241.2570784254 Correl. Energy= -1.0690445

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00027	0.00180	[YES]	0.00027	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.048294	-0.518013	-0.000002
C	-0.157671	-1.181347	-0.000045
N	0.646242	0.781594	0.000049
H	1.206292	1.624412	0.000097
H	2.079612	-0.830381	0.000008
N	-0.700324	0.897571	0.000038
N	-1.178724	-0.336004	-0.000061

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -240.188033917 Predicted Change= -1.575899D-08
MP2 Energy= -241.2570784254 MP2 Cor. Energy= -1.0690445
Zero-point correction (ZPE)= -241.4772 0.04626
Internal Energy (U)= -241.4736 0.04982
Enthalpy (H)= -241.4727 0.05077
Gibbs Free Energy (G)= -241.5039 0.01953

Frequencies -- 581.8439 612.2479 713.3502

Supporting Information: **5chloro123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -699.769350414 Predicted Change= -8.518930D-08
MP2 Energy= -701.4003558672 Correl. Energy= -1.63100545

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00048	0.00180	[YES]	0.00048	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.241480	0.081935	0.000002
C	-0.646176	1.133456	0.000090
N	-0.544276	-1.023093	-0.000067
H	-0.268348	-1.996074	-0.000128
H	-0.450128	2.194757	0.000169
N	-1.853252	-0.684488	0.000017
Cl	1.958387	0.007128	0.000021
N	-1.909034	0.620124	-0.000086

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -699.769350414 Predicted Change= -8.518930D-08
MP2 Energy= -701.4003558672 MP2 Cor. Energy= -1.63100545
Zero-point correction (ZPE)= -701.7608 0.04969
Internal Energy (U)= -701.7561 0.05434
Enthalpy (H)= -701.7552 0.05529
Gibbs Free Energy (G)= -701.7895 0.02101

Supporting Information: **5radical123triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -240.186584557 Predicted Change= -2.441715D-07
MP2 Energy= -241.2557274986 Correl. Energy= -1.06914294

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00047	0.00180	[YES]	0.00047	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.031884	-1.177019	-0.000014
C	1.134894	-0.360363	0.000051
N	-1.041936	-0.367624	-0.000001
H	-2.025466	-0.598536	-0.000037
H	2.187229	-0.593690	0.000155
N	-0.647515	0.931950	-0.000229
N	0.666247	0.923748	0.000182

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -240.186584557 Predicted Change= -2.441715D-07
MP2 Energy= -241.2557274986 MP2 Cor. Energy= -1.06914294
Zero-point correction (ZPE)= -241.4748 0.04619
Internal Energy (U)= -241.4712 0.04978
Enthalpy (H)= -241.4702 0.05073
Gibbs Free Energy (G)= -241.5015 0.01943

Frequencies -- 507.8546 614.1482 719.8555

Chlorooxadiazoles

Supporting Information: **3chloro124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -719.608160449 Predicted Change= -1.343531D-07
MP2 Energy= -721.2534641241 Correl. Energy= -1.64530367

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00052	0.00180	[YES]	0.00052	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.733483	0.646302	0.000009
C	0.218432	-0.003227	0.000103
H	-2.676768	1.175628	-0.000066
N	-0.442959	-1.134116	0.000060
O	-1.779144	-0.690249	0.000071
Cl	1.932155	0.024828	-0.000086
N	-0.535099	1.143521	-0.000018

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -719.608160449 Predicted Change= -1.343531D-07
MP2 Energy= -721.2534641241 MP2 Cor. Energy= -1.64530367
Zero-point correction (ZPE)= -721.6381 0.03713
Internal Energy (U)= -721.6337 0.04153
Enthalpy (H)= -721.6327 0.04247
Gibbs Free Energy (G)= -721.6666 0.00865

Frequencies -- 261.6553 332.9115 504.8612

Supporting Information: **3radical124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -260.024940986 Predicted Change= -1.841096D-07
MP2 Energy= -261.1265798345 Correl. Energy= -1.10163884

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00045	0.00180	[YES]	0.00045	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.920446	0.466294	-0.000075
C	0.440099	-1.041020	0.000031
H	-1.787721	1.113664	0.000040
N	1.244434	-0.033360	-0.000246
O	0.278709	1.054265	0.000178
N	-0.895845	-0.837987	0.000075

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -260.024940986 Predicted Change= -1.841096D-07
MP2 Energy= -261.1265798345 MP2 Cor. Energy= -1.10163884
Zero-point correction (ZPE)= -261.3548 0.03332
Internal Energy (U)= -261.3514 0.03678
Enthalpy (H)= -261.3504 0.03772
Gibbs Free Energy (G)= -261.3815 0.00663

Frequencies -- 593.2497 651.2468 692.3959

Supporting Information: **5chloro124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -719.608223713 Predicted Change= -2.555323D-07
MP2 Energy= -721.253271782 Correl. Energy= -1.64504806

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.206234	0.092088	-0.000177
C	1.791335	0.586009	-0.000169
N	1.828490	-0.720857	0.000173
H	2.701850	1.170580	0.000014
O	0.458981	-1.068991	-0.000030
Cl	-1.909007	0.016741	-0.000056
N	0.538484	1.153453	0.000292

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -719.608223713 Predicted Change= -2.555323D-07
MP2 Energy= -721.253271782 MP2 Cor. Energy= -1.64504806
Zero-point correction (ZPE)= -721.6377 0.03713
Internal Energy (U)= -721.6333 0.04154
Enthalpy (H)= -721.6323 0.04249
Gibbs Free Energy (G)= -721.6662 0.00864

Frequencies -- 245.0276 327.3837 511.0733

Supporting Information: **5radical124oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -260.024172056 Predicted Change= -3.446604D-07
MP2 Energy= -261.1284562221 Correl. Energy= -1.10428416

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00049	0.00180	[YES]	0.00049	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.350134	-1.055563	-0.000011
C	-0.889956	0.558297	0.000037
N	0.289957	1.121758	0.000005
H	-1.790021	1.159505	0.000049
O	1.171160	-0.029329	-0.000043
N	-0.910004	-0.827655	0.000015

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -260.024172056 Predicted Change= -3.446604D-07
MP2 Energy= -261.1284562221 MP2 Cor. Energy= -1.10428416
Zero-point correction (ZPE)= -261.3542 0.03339
Internal Energy (U)= -261.3508 0.03684
Enthalpy (H)= -261.3498 0.03778
Gibbs Free Energy (G)= -261.3809 0.00669

Frequencies -- 599.0670 633.8367 720.0565

Chlorotriazoles

Supporting Information: **3chloro124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2ClN3 C1[X(C2H2ClN3)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -699.809075718 Predicted Change= -5.503141D-07
MP2 Energy= -701.4298720307 Correl. Energy= -1.62079631

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.738224	0.704206	0.000063
C	-0.225201	0.006226	0.000035
N	1.737549	-0.645831	-0.000045
H	2.512158	-1.294664	-0.000121
H	2.637665	1.304650	0.000106
Cl	-1.948386	0.000717	-0.000001
N	0.465771	-1.123382	-0.000076
N	0.495908	1.157104	0.000043

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -699.809075718 Predicted Change= -5.503141D-07
MP2 Energy= -701.4298720307 MP2 Cor. Energy= -1.62079631
Zero-point correction (ZPE)= -701.7902 0.05037
Internal Energy (U)= -701.7856 0.05492
Enthalpy (H)= -701.7847 0.05587
Gibbs Free Energy (G)= -701.8187 0.02183

Frequencies -- 260.6478 336.3849 503.9062

Supporting Information: **3radical124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -240.224956454 Predicted Change= -1.306150D-07
MP2 Energy= -241.304202104 Correl. Energy= -1.07924565

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.713912	0.783427	-0.000090
C	-0.003667	-1.151326	-0.000006
N	-0.637437	0.802165	0.000079
H	-1.274163	1.587582	0.000159
H	1.325279	1.675937	-0.000131
N	-1.129246	-0.480980	0.000004
N	1.150599	-0.472061	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -240.224956454 Predicted Change= -1.306150D-07
MP2 Energy= -241.304202104 MP2 Cor. Energy= -1.07924565
Zero-point correction (ZPE)= -241.5047 0.04680
Internal Energy (U)= -241.5011 0.05036
Enthalpy (H)= -241.5002 0.05131
Gibbs Free Energy (G)= -241.5314 0.02007

Frequencies -- 517.4302 647.4172 672.0637

Supporting Information: **5chloro124triazole.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # g3b3
 #N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
 #N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
 #N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C2H2ClN3   C1[X(C2H2ClN3)]  #Atoms= 8
 Charge = 0     Multiplicity = 1
---------------------------------------------------------------------
 SCF Energy= -699.808720889     Predicted Change= -7.420284D-07
 MP2 Energy= -701.4295231225     Correl. Energy= -1.62080223
=====================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00037 ||  0.00045   [ YES ]      0.00013 ||  0.00030   [ YES ]
 Displ      0.00076 ||  0.00180   [ YES ]      0.00076 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type       X          Y       Z
---------------------------------------------------------------------
      C        0.217301      -0.084068       0.000007
      C       -1.792176      -0.629191       0.000064
      N       -0.541794       1.033936       0.000054
      H       -0.255388       2.002835       0.000105
      N       -1.857101       0.694168       0.000046
      H       -2.683707      -1.240715       0.000043
      Cl       1.936253      -0.026379      -0.000032
      N       -0.533671      -1.161551      -0.000104
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -699.808720889 Predicted Change= -7.420284D-07
 MP2 Energy=     -701.4295231225        MP2 Cor. Energy= -1.62080223
 Zero-point correction (ZPE)=         -701.7896  0.05046
 Internal Energy (U)=                 -701.7850  0.05505
 Enthalpy (H)=                        -701.7841   0.05600
 Gibbs Free Energy (G)=               -701.8182    0.02187
---------------------------------------------------------------------
 Frequencies --   248.5808              318.4567              500.2053
```

Supporting Information: **5radical124triazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2H2N3(2) C1[X(C2H2N3)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -240.224542887 Predicted Change= -8.991566D-08
MP2 Energy= -241.3050413938 Correl. Energy= -1.0804985

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00039	0.00180	[YES]	0.00039	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.217386	-1.127373	0.000029
C	0.853627	0.644159	0.000072
N	-1.094689	-0.109860	0.000030
H	-2.103350	-0.114211	0.000015
N	-0.399019	1.073603	-0.000198
H	1.689977	1.329341	0.000076
N	1.007412	-0.723150	0.000068

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -240.224542887 Predicted Change= -8.991566D-08
MP2 Energy= -241.3050413938 MP2 Cor. Energy= -1.0804985
Zero-point correction (ZPE)= -241.5057 0.04701
Internal Energy (U)= -241.5021 0.05061
Enthalpy (H)= -241.5011 0.05155
Gibbs Free Energy (G)= -241.5324 0.02025

Frequencies -- 457.6395 637.0827 684.0356

Chlorooxadiazoles

Supporting Information: **3chloro125oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -719.550585676 Predicted Change= -3.695128D-07
MP2 Energy= -721.2120601195 Correl. Energy= -1.66147444

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00021	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00150	0.00180	[YES]	0.00150	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.645557	1.106772	0.000008
C	-0.238899	-0.011300	-0.000068
H	0.419660	2.163179	0.000065
N	0.452670	-1.119592	0.000177
O	1.762246	-0.710507	-0.000265
Cl	-1.954290	0.009218	0.000015
N	1.870952	0.661212	0.000132

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -719.550585676 Predicted Change= -3.695128D-07
MP2 Energy= -721.2120601195 MP2 Cor. Energy= -1.66147444
Zero-point correction (ZPE)= -721.5982 0.03640
Internal Energy (U)= -721.5937 0.04088
Enthalpy (H)= -721.5928 0.04182
Gibbs Free Energy (G)= -721.6268 0.00784

Frequencies -- 266.1597 308.9122 495.9115

Supporting Information: **3radical125oxadiazole3.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcycle=5000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -259.974941195 Predicted Change= -6.994238D-07
MP2 Energy= -261.0561655643 Correl. Energy= -1.08122436

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00133	0.00180	[YES]	0.00133	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.080847	0.423133	-0.000018
C	-0.138586	1.159706	0.000264
H	2.106514	0.759071	0.000081
N	-1.167837	0.401097	-0.000317
O	-0.615949	-0.894613	0.000224
N	0.763195	-0.843841	-0.000161

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -259.974941195 Predicted Change= -6.994238D-07
MP2 Energy= -261.0561655643 MP2 Cor. Energy= -1.08122436
Zero-point correction (ZPE)= -261.3148 0.03261
Internal Energy (U)= -261.3113 0.03611
Enthalpy (H)= -261.3103 0.03705
Gibbs Free Energy (G)= -261.3415 0.00588

Frequencies -- 591.1112 637.7531 718.0781

Supporting Information: **2chloro134oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HClN2O C1[X(C2HClN2O)] #Atoms= 7
Charge = 0 Multiplicity = 1

SCF Energy= -719.619063486 Predicted Change= -6.089712D-07
MP2 Energy= -721.2628348498 Correl. Energy= -1.64377136

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00164	0.00180	[YES]	0.00164	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.211887	0.095012	-0.000033
C	1.777614	-0.582860	0.000119
H	2.583853	-1.300493	0.000194
N	1.841079	0.705928	0.000100
O	0.501438	-1.061967	0.000075
Cl	-1.910338	-0.020859	-0.000120
N	0.514068	1.162345	0.000004

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -719.619063486 Predicted Change= -6.089712D-07
MP2 Energy= -721.2628348498 MP2 Cor. Energy= -1.64377136
Zero-point correction (ZPE)= -721.6443 0.03697
Internal Energy (U)= -721.6398 0.04141
Enthalpy (H)= -721.6389 0.04235
Gibbs Free Energy (G)= -721.6728 0.00847

Frequencies -- 243.5394 326.5868 510.0765

Supporting Information: **2radical134oxadiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C2HN2O(2) C1[X(C2HN2O)] #Atoms= 6
Charge = 0 Multiplicity = 2

SCF Energy= -260.035087742 Predicted Change= -8.383368D-07
MP2 Energy= -261.1303963516 Correl. Energy= -1.09530861

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00044	0.00045	[YES]	0.00017	0.00030	[YES]
Displ	0.00117	0.00180	[YES]	0.00117	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.477923	-1.013511	-0.000103
C	0.859976	0.584073	-0.000002
H	1.815295	1.087017	0.000105
N	-0.321748	1.105787	0.000121
O	0.853087	-0.785555	0.000064
N	-1.240011	0.004792	-0.000119

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -260.035087742 Predicted Change= -8.383368D-07
MP2 Energy= -261.1303963516 MP2 Cor. Energy= -1.09530861
Zero-point correction (ZPE)= -261.3588 0.03315
Internal Energy (U)= -261.3554 0.03661
Enthalpy (H)= -261.3544 0.03755
Gibbs Free Energy (G)= -261.3855 0.00647

Frequencies -- 574.9892 641.6295 833.1917

Chlorofurans

Supporting Information: **23dichlorofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2Cl2O C1[X(C4H2Cl2O)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1146.55067865 Predicted Change= -6.162684D-07
MP2 Energy= -1148.611160418 Correl. Energy= -2.06048176

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00042	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00141	0.00180	[YES]	0.00141	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.649092	0.028450	-0.000073
C	-0.697380	0.249301	0.000013
C	-0.874664	1.671956	-0.000303
C	0.376980	2.199090	0.000290
H	-1.815014	2.203330	-0.000463
H	0.764712	3.205584	0.000568
O	1.320659	1.207641	-0.000078
Cl	1.577097	-1.406114	-0.000008
Cl	-1.944106	-0.944640	0.000065

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1146.55067865 Predicted Change= -6.162684D-07
MP2 Energy= -1148.611160418 MP2 Cor. Energy= -2.06048176
Zero-point correction (ZPE)= -1149.1501 0.05145
Internal Energy (U)= -1149.1442 0.05736
Enthalpy (H)= -1149.1432 0.05830
Gibbs Free Energy (G)= -1149.1811 0.02040

Frequencies -- 166.9348 200.4054 254.4009

Supporting Information: **24dichlorofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2Cl2O C1[X(C4H2Cl2O)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1146.55165792 Predicted Change= -6.096069D-08
MP2 Energy= -1148.610881277 Correl. Energy= -2.05922335

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.631204	1.319496	0.000174
C	1.125573	0.052123	-0.000157
C	0.012355	-0.850998	0.000257
C	-1.080943	-0.040951	0.000150
H	1.078239	2.300039	0.000218
H	0.034860	-1.929805	0.000357
O	-0.737616	1.270488	0.000205
Cl	2.798390	-0.396672	-0.000524
Cl	-2.759644	-0.392278	0.000244

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1146.55165792 Predicted Change= -6.096069D-08
MP2 Energy= -1148.610881277 MP2 Cor. Energy= -2.05922335
Zero-point correction (ZPE)= -1149.1512 0.05132
Internal Energy (U)= -1149.1453 0.05725
Enthalpy (H)= -1149.1444 0.05819
Gibbs Free Energy (G)= -1149.1823 0.02027

Frequencies -- 145.9446 201.4909 308.4874

Supporting Information: **2chloro3radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -686.969861376 Predicted Change= -4.911396D-08
MP2 Energy= -688.4713615115 Correl. Energy= -1.50150013

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00045	0.00180	[YES]	0.00045	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.255939	-0.146321	0.000030
C	0.607079	-1.185970	-0.000005
C	1.937486	-0.679468	-0.000015
C	1.779364	0.675311	0.000037
H	2.867145	-1.229349	-0.000031
H	2.470287	1.504601	0.000057
O	0.453122	1.023979	-0.000042
Cl	-1.962962	-0.026377	0.000002

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -686.969861376 Predicted Change= -4.911396D-08
MP2 Energy= -688.4713615115 MP2 Cor. Energy= -1.50150013
Zero-point correction (ZPE)= -688.8630 0.04815
Internal Energy (U)= -688.8583 0.05290
Enthalpy (H)= -688.8574 0.05384
Gibbs Free Energy (G)= -688.8924 0.01882

Frequencies -- 208.4965 313.5255 494.5055

Supporting Information: **2chloro4radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -686.971054267 Predicted Change= -1.161144D-06
MP2 Energy= -688.4739790099 Correl. Energy= -1.50292474

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00155	0.00180	[YES]	0.00155	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.869702	-0.640750	0.000176
C	1.910928	0.707896	-0.000216
C	0.591811	1.241655	0.000162
C	-0.190579	0.122156	-0.000062
H	2.590671	-1.440916	0.000181
H	0.263623	2.269458	0.000197
O	0.538654	-1.022430	0.000215
Cl	-1.897335	-0.072638	-0.000145

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -686.971054267 Predicted Change= -1.161144D-06
MP2 Energy= -688.4739790099 MP2 Cor. Energy= -1.50292474
Zero-point correction (ZPE)= -688.8651 0.04807
Internal Energy (U)= -688.8604 0.05282
Enthalpy (H)= -688.8594 0.05376
Gibbs Free Energy (G)= -688.8944 0.01876

Frequencies -- 222.9401 315.0044 488.9690

Supporting Information: **2chlorofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

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g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClO C1[X(C4H3ClO)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -687.627026432 Predicted Change= -8.296748D-08
MP2 Energy= -689.1966452151 Correl. Energy= -1.56961878

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.245110	0.103410	0.000031
C	0.595975	1.173034	-0.000260
C	1.918080	0.613205	0.000225
C	1.766282	-0.737739	0.000015
H	0.312792	2.215033	-0.000420
H	2.852926	1.156138	0.000467
H	2.449007	-1.572893	0.000069
O	0.436357	-1.068887	-0.000182
Cl	-1.959821	-0.009332	0.000075

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -687.627026432 Predicted Change= -8.296748D-08
MP2 Energy= -689.1966452151 MP2 Cor. Energy= -1.56961878
Zero-point correction (ZPE)= -689.5512 0.06078
Internal Energy (U)= -689.5465 0.06554
Enthalpy (H)= -689.5455 0.06648
Gibbs Free Energy (G)= -689.5799 0.03207

Frequencies -- 222.7153 313.0202 490.6118

Supporting Information: **2radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3O(2) C1[X(C4H3O)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -228.045359123 Predicted Change= -2.835661D-07
MP2 Energy= -229.060710079 Correl. Energy= -1.01535095

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00108	0.00180	[YES]	0.00108	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.209676	-1.162281	-0.000036
C	-1.208803	-0.243201	0.000284
C	-0.506563	1.020116	-0.000384
C	0.824181	0.740200	0.000413
H	-2.273712	-0.416412	0.000422
H	-0.954882	2.004748	-0.000699
H	1.725914	1.332073	0.000704
O	1.013481	-0.631177	-0.000261

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -228.045359123 Predicted Change= -2.835661D-07
MP2 Energy= -229.060710079 MP2 Cor. Energy= -1.01535095
Zero-point correction (ZPE)= -229.2641 0.05714
Internal Energy (U)= -229.2603 0.06089
Enthalpy (H)= -229.2594 0.06184
Gibbs Free Energy (G)= -229.2909 0.03027

Frequencies -- 479.6383 605.9435 702.9918

Supporting Information: **3chloro2radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -686.969414484 Predicted Change= -5.297178D-08
MP2 Energy= -688.4701978008 Correl. Energy= -1.50078331

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00027	0.00180	[YES]	0.00027	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.546552	-1.117171	0.000202
C	-0.283503	-0.040872	-0.000067
C	0.597895	1.101225	0.000080
C	1.864256	0.607502	0.000082
H	0.297714	2.139663	0.000025
H	2.847792	1.050166	0.000086
O	1.833997	-0.774979	0.000384
Cl	-2.009923	-0.017300	-0.000292

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -686.969414484 Predicted Change= -5.297178D-08
MP2 Energy= -688.4701978008 MP2 Cor. Energy= -1.50078331
Zero-point correction (ZPE)= -688.8621 0.04790
Internal Energy (U)= -688.8573 0.05271
Enthalpy (H)= -688.8563 0.05365
Gibbs Free Energy (G)= -688.8915 0.01849

Frequencies -- 229.7544 298.2985 457.2052

Supporting Information: **3chlorofuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClO C1[X(C4H3ClO)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -687.626797921 Predicted Change= -1.352037D-07
MP2 Energy= -689.1954539019 Correl. Energy= -1.56865598

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00128	0.00180	[YES]	0.00128	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.525881	-1.098090	0.000361
C	-0.274422	0.003460	-0.000058
C	0.580454	1.153289	0.000489
C	1.846168	0.655554	-0.000370
H	0.332664	-2.158765	0.000558
H	0.277931	2.190131	0.000840
H	2.823557	1.113060	-0.000733
O	1.831382	-0.707915	-0.000117
Cl	-2.009041	0.013742	-0.000133

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -687.626797921 Predicted Change= -1.352037D-07
MP2 Energy= -689.1954539019 MP2 Cor. Energy= -1.56865598
Zero-point correction (ZPE)= -689.5512 0.06091
Internal Energy (U)= -689.5464 0.06567
Enthalpy (H)= -689.5455 0.06662
Gibbs Free Energy (G)= -689.5799 0.03217

Frequencies -- 249.9133 294.0003 476.6580

Supporting Information: **3radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3O(2) C1[X(C4H3O)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -228.044928444 Predicted Change= -4.967048D-08
MP2 Energy= -229.0602240776 Correl. Energy= -1.01529563

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00031	0.00180	[YES]	0.00031	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.139341	-0.352072	0.000078
C	0.108446	-1.225981	-0.000038
C	-1.124428	-0.513867	-0.000013
C	-0.743097	0.796785	0.000061
H	2.214167	-0.427485	0.000072
H	-2.132148	-0.902626	-0.000027
H	-1.293363	1.726029	0.000102
O	0.616221	0.921861	-0.000083

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -228.044928444 Predicted Change= -4.967048D-08
MP2 Energy= -229.0602240776 MP2 Cor. Energy= -1.01529563
Zero-point correction (ZPE)= -229.2641 0.05752
Internal Energy (U)= -229.2604 0.06122
Enthalpy (H)= -229.2595 0.06216
Gibbs Free Energy (G)= -229.2910 0.03067

Frequencies -- 546.2086 616.7266 695.7238

Supporting Information: **4chloro2radicalfuran.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClO(2) C1[X(C4H2ClO)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -686.971055475 Predicted Change= -1.550099D-07
MP2 Energy= -688.473618643 Correl. Energy= -1.50256316

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00085	0.00180	[YES]	0.00085	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.617923	-1.059779	0.000348
C	0.216959	0.015163	0.000001
C	-0.584519	1.215784	0.000236
C	-1.850027	0.727464	-0.000434
H	-0.477987	-2.128250	0.000620
H	-0.246801	2.239668	0.000431
O	-1.923289	-0.602061	-0.000602
Cl	1.948480	-0.040395	0.000168

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -686.971055475 Predicted Change= -1.550099D-07
MP2 Energy= -688.473618643 MP2 Cor. Energy= -1.50256316
Zero-point correction (ZPE)= -688.8650 0.04787
Internal Energy (U)= -688.8602 0.05266
Enthalpy (H)= -688.8592 0.05360
Gibbs Free Energy (G)= -688.8943 0.01851

Frequencies -- 247.7103 297.0466 475.5895

Supporting Information: **furan.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H4O C1[X(C4H4O)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -228.701194033 Predicted Change= -2.709721D-07
MP2 Energy= -229.7807464229 Correl. Energy= -1.07955239

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00113	0.00180	[YES]	0.00113	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.095472	-0.346219	0.000294
C	0.716765	0.960688	-0.000277
C	-0.718925	0.959245	0.000312
C	-1.094445	-0.348566	-0.000297
H	1.371434	1.821099	-0.000490
H	-1.375553	1.818176	0.000552
H	-2.049141	-0.852046	-0.000518
O	0.001122	-1.161278	-0.000030
H	2.051087	-0.847893	0.000505

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -228.701194033 Predicted Change= -2.709721D-07
MP2 Energy= -229.7807464229 MP2 Cor. Energy= -1.07955239
Zero-point correction (ZPE)= -229.9503 0.07019
Internal Energy (U)= -229.9466 0.07391
Enthalpy (H)= -229.9457 0.07485
Gibbs Free Energy (G)= -229.9766 0.04392

Frequencies -- 613.8597 622.9856 722.3701

Chloroimidazoles

Supporting Information: 24dichloroimidazole.out

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2Cl2N2 C1[X(C3H2Cl2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1142.74392049 Predicted Change= -5.543113D-07
MP2 Energy= -1144.816067934 Correl. Energy= -2.07214744

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00096	0.00180	[YES]	0.00096	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.029364	0.001781	0.000019
C	-1.079545	0.083520	0.000012
C	-0.677501	1.394487	0.000208
N	0.705293	1.324729	0.000019
H	1.354420	2.098827	0.000039
H	-1.218805	2.326852	0.000341
N	-0.017893	-0.781288	-0.000070
Cl	2.676570	-0.511257	-0.000056
Cl	-2.710766	-0.495125	-0.000029

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1142.74392049 Predicted Change= -5.543113D-07
MP2 Energy= -1144.816067934 MP2 Cor. Energy= -2.07214744
Zero-point correction (ZPE)= -1145.3476 0.05224
Internal Energy (U)= -1145.3417 0.05820
Enthalpy (H)= -1145.3407 0.05914
Gibbs Free Energy (G)= -1145.3786 0.02123

Frequencies -- 162.2062 207.0136 295.3931

Supporting Information: **25dichloroimidazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2Cl2N2 C1[X(C3H2Cl2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1142.74143432 Predicted Change= -1.596270D-07
MP2 Energy= -1144.813390556 Correl. Energy= -2.07195623

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00130 ‖	0.00180	[YES]	0.00130 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.084565	0.160404	-0.000160
C	0.625267	1.436269	0.000399
C	1.104917	0.153833	0.000029
N	-0.002595	-0.673259	0.000647
H	-0.004844	-1.683588	0.001051
N	-0.755778	1.422216	-0.000097
Cl	-2.689236	-0.477170	-0.000381
H	1.185225	2.359882	0.000569
Cl	2.704207	-0.488832	-0.000035

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1142.74143432 Predicted Change= -1.596270D-07
MP2 Energy= -1144.813390556 MP2 Cor. Energy= -2.07195623
Zero-point correction (ZPE)= -1145.3451 0.05231
Internal Energy (U)= -1145.3391 0.05832
Enthalpy (H)= -1145.3382 0.05926
Gibbs Free Energy (G)= -1145.3762 0.02122

Frequencies -- 154.8609 197.3673 286.1868

Supporting Information: **2chloro4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -683.160077689 Predicted Change= -3.136227D-07
MP2 Energy= -684.6898367949 Correl. Energy= -1.5297591

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00137	0.00180	[YES]	0.00137	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.179101	-0.103128	-0.000191
C	1.787542	-0.823168	0.000096
C	1.937915	0.535921	-0.000586
N	0.622525	0.998429	0.000579
H	0.307864	1.959325	0.001026
H	2.787665	1.198694	-0.000915
N	0.508966	-1.223910	0.000305
Cl	-1.899653	0.044858	-0.000130

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.160077689 Predicted Change= -3.136227D-07
MP2 Energy= -684.6898367949 MP2 Cor. Energy= -1.5297591
Zero-point correction (ZPE)= -685.0629 0.04913
Internal Energy (U)= -685.0582 0.05391
Enthalpy (H)= -685.0572 0.05485
Gibbs Free Energy (G)= -685.0922 0.01984

Frequencies -- 233.9866 324.1607 492.4491

Supporting Information: **2chloro5radicalimidazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -683.156662158 Predicted Change= -3.087396D-07
MP2 Energy= -684.6844618854 Correl. Energy= -1.52779972

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00156	0.00180	[YES]	0.00156	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.173743	-0.053689	0.000039
C	-1.906803	-0.618014	0.000033
C	-1.847821	0.744291	0.000155
N	-0.525083	1.120132	0.000019
H	-0.151191	2.057890	0.000049
N	-0.604723	-1.103199	-0.000195
Cl	1.900244	-0.078412	-0.000012
H	-2.759026	-1.278948	0.000009

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.156662158 Predicted Change= -3.087396D-07
MP2 Energy= -684.6844618854 MP2 Cor. Energy= -1.52779972
Zero-point correction (ZPE)= -685.0589 0.04897
Internal Energy (U)= -685.0541 0.05383
Enthalpy (H)= -685.0531 0.05477
Gibbs Free Energy (G)= -685.0883 0.01960

Frequencies -- 223.8572 320.1736 419.8859

Supporting Information: **2chloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -683.817568197 Predicted Change= -2.335899D-07
MP2 Energy= -685.3994051953 Correl. Energy= -1.58183699

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00112	0.00180	[YES]	0.00112	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.224293	-0.087193	-0.000032
C	-1.804522	-0.717410	0.000072
C	-1.847508	0.652692	0.000126
N	-0.523480	1.054059	0.000125
H	-0.168646	1.999253	0.000264
H	-2.632900	-1.412040	0.000077
H	-2.660483	1.362749	0.000194
N	-0.499749	-1.172474	-0.000033
Cl	1.952415	-0.012329	-0.000128

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.817568197 Predicted Change= -2.335899D-07
MP2 Energy= -685.3994051953 MP2 Cor. Energy= -1.58183699
Zero-point correction (ZPE)= -685.7456 0.06178
Internal Energy (U)= -685.7408 0.06660
Enthalpy (H)= -685.7398 0.06755
Gibbs Free Energy (G)= -685.7743 0.03307

Frequencies -- 233.0408 320.1598 492.2728

Supporting Information: **2radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -224.233808279 Predicted Change= -6.251043D-07
MP2 Energy= -225.2768138881 Correl. Energy= -1.0430056

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00036	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00079	0.00180	[YES]	0.00079	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.084240	-1.164306	-0.000079
C	0.852437	0.740002	0.000214
C	-0.494517	0.992258	-0.000235
N	-1.101806	-0.263463	0.000150
H	-2.090428	-0.462747	0.000217
H	1.672341	1.444593	0.000386
H	-1.068042	1.907567	-0.000394
N	1.079527	-0.636128	-0.000094

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -224.233808279 Predicted Change= -6.251043D-07
MP2 Energy= -225.2768138881 MP2 Cor. Energy= -1.0430056
Zero-point correction (ZPE)= -225.4620 0.05827
Internal Energy (U)= -225.4582 0.06212
Enthalpy (H)= -225.4572 0.06306
Gibbs Free Energy (G)= -225.4889 0.03136

Frequencies -- 417.9161 582.3490 624.8687

Supporting Information: **45dichloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2Cl2N2 C1[X(C3H2Cl2N2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1142.74049372 Predicted Change= -4.811747D-07
MP2 Energy= -1144.814212099 Correl. Energy= -2.07371837

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013 ‖	0.00045	[YES]	0.00003 ‖	0.00030	[YES]
Displ	0.00171 ‖	0.00180	[YES]	0.00171 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.126514	2.195950	0.000717
C	0.700751	0.230938	0.000156
C	-0.663163	0.059488	0.000066
N	-1.186914	1.335750	-0.000352
H	-2.171139	1.565459	-0.000697
N	1.024111	1.556623	-0.000668
Cl	-1.657718	-1.340313	0.000025
H	-0.249997	3.270046	0.001013
Cl	1.898560	-1.012650	0.000045

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1142.74049372 Predicted Change= -4.811747D-07
MP2 Energy= -1144.814212099 MP2 Cor. Energy= -2.07371837
Zero-point correction (ZPE)= -1145.3449 0.05247
Internal Energy (U)= -1145.3389 0.05843
Enthalpy (H)= -1145.3380 0.05938
Gibbs Free Energy (G)= -1145.3760 0.02140

Frequencies -- 166.4685 202.2407 258.3255

Supporting Information: **4chloro2radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -683.160719916 Predicted Change= -1.203581D-07
MP2 Energy= -684.6919892497 Correl. Energy= -1.53126933

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.715931	-0.855519	0.000005
C	0.210512	-0.009965	-0.000057
C	-0.645116	1.061342	0.000320
N	-1.915972	0.485548	-0.000258
H	-2.800942	0.970363	-0.000479
H	-0.479892	2.127427	0.000526
N	-0.482644	-1.205713	0.000205
Cl	1.939668	0.045189	-0.000076

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.160719916 Predicted Change= -1.203581D-07
MP2 Energy= -684.6919892497 MP2 Cor. Energy= -1.53126933
Zero-point correction (ZPE)= -685.0644 0.04891
Internal Energy (U)= -685.0596 0.05377
Enthalpy (H)= -685.0586 0.05471
Gibbs Free Energy (G)= -685.0938 0.01955

Frequencies -- 249.1540 320.3538 415.2651

Supporting Information: **4chloro5radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -683.155465742 Predicted Change= -7.649637D-07
MP2 Energy= -684.6811155955 Correl. Energy= -1.52564985

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00044	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00169	0.00180	[YES]	0.00169	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.746120	0.708407	0.000586
C	0.268432	-0.050590	0.000162
C	-0.565572	-1.131927	0.000030
N	-1.851335	-0.654226	-0.000287
H	-2.694849	-1.209634	-0.000579
N	-0.484222	1.095169	-0.000275
H	-2.601788	1.369353	0.000843
Cl	1.994417	-0.023627	-0.000058

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -683.155465742 Predicted Change= -7.649637D-07
MP2 Energy= -684.6811155955 MP2 Cor. Energy= -1.52564985
Zero-point correction (ZPE)= -685.0575 0.04897
Internal Energy (U)= -685.0526 0.05384
Enthalpy (H)= -685.0516 0.05479
Gibbs Free Energy (G)= -685.0869 0.01957

Frequencies -- 220.7571 322.1891 401.4022

Supporting Information: **4chloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -683.817657537 Predicted Change= -2.269306D-07
MP2 Energy= -685.4000968233 Correl. Energy= -1.58243928

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00130	0.00180	[YES]	0.00130	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.724542	-0.763293	-0.000088
C	-0.254940	0.002756	0.000017
C	0.551919	1.113817	0.000047
N	1.832209	0.597351	0.000065
H	2.688278	1.133290	0.000206
H	2.586438	-1.416390	-0.000155
H	0.339688	2.170853	0.000102
N	0.466791	-1.155053	-0.000125
Cl	-1.990384	-0.006089	0.000024

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.817657537 Predicted Change= -2.269306D-07
MP2 Energy= -685.4000968233 MP2 Cor. Energy= -1.58243928
Zero-point correction (ZPE)= -685.7467 0.06186
Internal Energy (U)= -685.7419 0.06666
Enthalpy (H)= -685.7409 0.06761
Gibbs Free Energy (G)= -685.7754 0.03316

Frequencies -- 249.3283 317.1711 483.8617

Supporting Information: **4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -224.233079166 Predicted Change= -4.626796D-07
MP2 Energy= -225.274162051 Correl. Energy= -1.04108288

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00136	0.00180	[YES]	0.00136	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.821094	0.703313	0.000175
C	-0.077738	-1.206713	-0.000215
C	-1.139620	-0.341794	0.000322
N	-0.528402	0.907863	-0.000091
H	-0.995774	1.804319	-0.000113
H	1.536434	1.514591	0.000258
H	-2.209865	-0.469140	0.000520
N	1.106515	-0.590521	-0.000246

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -224.233079166 Predicted Change= -4.626796D-07
MP2 Energy= -225.274162051 MP2 Cor. Energy= -1.04108288
Zero-point correction (ZPE)= -225.4614 0.05857
Internal Energy (U)= -225.4577 0.06231
Enthalpy (H)= -225.4567 0.06325
Gibbs Free Energy (G)= -225.4883 0.03174

Frequencies -- 524.5465 599.9321 671.5358

Supporting Information: **5chloro2radicalimidazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -683.158503497 Predicted Change= -2.879330D-07
MP2 Energy= -684.6898172134 Correl. Energy= -1.53131371

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00131	0.00180	[YES]	0.00131	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.849585	0.693508	-0.000501
C	0.701560	-1.104298	0.000500
C	-0.196189	-0.070552	-0.000073
N	0.552931	1.103887	0.000555
H	0.194378	2.047292	0.000969
N	1.990823	-0.575500	-0.000678
H	0.511045	-2.167273	0.000843
Cl	-1.920084	-0.040628	-0.000030

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.158503497 Predicted Change= -2.879330D-07
MP2 Energy= -684.6898172134 MP2 Cor. Energy= -1.53131371
Zero-point correction (ZPE)= -685.0629 0.04895
Internal Energy (U)= -685.0580 0.05386
Enthalpy (H)= -685.0571 0.05481
Gibbs Free Energy (G)= -685.0924 0.01952

Frequencies -- 230.5840 300.7706 400.6941

Supporting Information: **5chloro4radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClN2(2) C1[X(C3H2ClN2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -683.156484261 Predicted Change= -1.802430D-07
MP2 Energy= -684.6842148375 Correl. Energy= -1.52773057

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00111	0.00180	[YES]	0.00111	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.850149	0.555233	0.000247
C	0.627200	-1.176297	-0.000151
C	-0.251592	-0.128996	0.000014
N	0.558267	0.999028	0.000015
H	0.238596	1.958708	-0.000075
N	1.895843	-0.768345	0.000410
Cl	-1.968876	-0.017541	-0.000235
H	2.698982	1.225068	0.000425

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.156484261 Predicted Change= -1.802430D-07
MP2 Energy= -684.6842148375 MP2 Cor. Energy= -1.52773057
Zero-point correction (ZPE)= -685.0600 0.04931
Internal Energy (U)= -685.0552 0.05410
Enthalpy (H)= -685.0542 0.05504
Gibbs Free Energy (G)= -685.0893 0.01996

Frequencies -- 223.6661 305.4350 488.6244

Supporting Information: **5chloroimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -683.814814461 Predicted Change= -2.358405D-07
MP2 Energy= -685.3970854529 Correl. Energy= -1.58227099

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00199	0.00180	[NO]	0.00199	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.833526	-0.616490	0.000184
C	0.613868	1.150877	0.000077
C	-0.249931	0.086255	-0.000017
N	0.534302	-1.046853	-0.000006
H	0.196879	-1.998962	-0.000150
H	2.668082	-1.304663	0.000272
H	0.371364	2.203846	0.000093
N	1.913556	0.695607	0.000094
Cl	-1.973889	-0.009726	-0.000135

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.814814461 Predicted Change= -2.358405D-07
MP2 Energy= -685.3970854529 MP2 Cor. Energy= -1.58227099
Zero-point correction (ZPE)= -685.7437 0.06190
Internal Energy (U)= -685.7388 0.06675
Enthalpy (H)= -685.7379 0.06769
Gibbs Free Energy (G)= -685.7725 0.03312

Frequencies -- 227.7798 297.5444 485.5304

Supporting Information: **5radicalimidazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -224.229325133 Predicted Change= -2.486471D-07
MP2 Energy= -225.2679354011 Correl. Energy= -1.03861026

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00117	0.00180	[YES]	0.00117	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.707613	0.812363	0.000376
C	-1.188652	-0.244499	0.000144
C	-0.192624	-1.179134	0.000186
N	1.012081	-0.521578	-0.000191
H	1.927316	-0.947164	-0.000368
H	1.460354	1.589235	0.000492
H	-2.259753	-0.373845	0.000128
N	-0.595787	1.007206	-0.000451

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -224.229325133 Predicted Change= -2.486471D-07
MP2 Energy= -225.2679354011 MP2 Cor. Energy= -1.03861026
Zero-point correction (ZPE)= -225.4568 0.05844
Internal Energy (U)= -225.4530 0.06223
Enthalpy (H)= -225.4520 0.06318
Gibbs Free Energy (G)= -225.4837 0.03155

Frequencies -- 434.4923 556.2799 679.1738

Chloroisothiazoles

Supporting Information: **35dichloroisothiazole2.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1485.22260890 Predicted Change= -4.151368D-07
MP2 Energy= -1487.52238441 Correl. Energy= -2.29977551

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00026	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00101	0.00180	[YES]	0.00101	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.198684	-0.026305	0.000159
C	0.094551	-0.930741	0.000184
C	-1.062785	-0.202817	-0.000023
S	-0.699247	1.495648	0.000344
H	0.168040	-2.009349	0.000199
N	0.964296	1.259814	-0.000242
Cl	2.847459	-0.592852	-0.000166
Cl	-2.677627	-0.806003	-0.000183

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1485.22260890 Predicted Change= -4.151368D-07
MP2 Energy= -1487.52238441 MP2 Cor. Energy= -2.29977551
Zero-point correction (ZPE)= -1488.1875 0.03632
Internal Energy (U)= -1488.1813 0.04251
Enthalpy (H)= -1488.1803 0.04345
Gibbs Free Energy (G)= -1488.2192 0.00456

Frequencies -- 156.8885 189.2989 275.2450

Supporting Information: **3chloro5radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64698251 Predicted Change= -4.672559D-07
MP2 Energy= -1027.38636207 Correl. Energy= -1.73937956

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00095	0.00180	[YES]	0.00095	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.501128	0.053891	-0.000283
C	0.092050	1.357585	-0.000025
C	1.437482	1.164080	0.000747
S	1.888842	-0.479339	-0.000326
H	-0.444117	2.296327	0.000173
N	0.274190	-1.003625	0.000482
Cl	-2.227477	-0.179698	-0.000057

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64698251 Predicted Change= -4.672559D-07
MP2 Energy= -1027.38636207 MP2 Cor. Energy= -1.73937956
Zero-point correction (ZPE)= -1027.9072 0.03320
Internal Energy (U)= -1027.9022 0.03816
Enthalpy (H)= -1027.9013 0.03911
Gibbs Free Energy (G)= -1027.9372 0.00313

Frequencies -- 223.9805 301.0024 427.8377

Supporting Information: **3chloroisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1026.30057239 Predicted Change= -9.211125D-08
MP2 Energy= -1028.10858143 Correl. Energy= -1.80800904

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00067	0.00180	[YES]	0.00067	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.533395	0.028120	-0.000137
C	0.120646	1.298513	0.000044
C	1.473385	1.107517	0.000033
S	1.813375	-0.584866	-0.000053
H	-0.390058	2.252377	0.000076
H	2.255982	1.855667	0.000057
N	0.200011	-1.053874	0.000179
Cl	-2.273166	-0.116351	-0.000011

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1026.30057239 Predicted Change= -9.211125D-08
MP2 Energy= -1028.10858143 MP2 Cor. Energy= -1.80800904
Zero-point correction (ZPE)= -1028.5895 0.04574
Internal Energy (U)= -1028.5845 0.05072
Enthalpy (H)= -1028.5836 0.05167
Gibbs Free Energy (G)= -1028.6189 0.01629

Frequencies -- 220.9576 302.8591 433.4311

Supporting Information: **3radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -566.724291848 Predicted Change= -2.319017D-07
MP2 Energy= -567.9797246302 Correl. Energy= -1.25543278

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00085	0.00180	[YES]	0.00085	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.970791	1.027489	-0.000003
C	-1.452713	-0.314444	-0.000003
C	-0.363428	-1.145684	0.000031
S	1.105251	-0.227560	-0.000037
H	-2.490082	-0.619958	-0.000029
H	-0.352497	-2.229299	0.000028
N	0.268593	1.298007	0.000062

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -566.724291848 Predicted Change= -2.319017D-07
MP2 Energy= -567.9797246302 MP2 Cor. Energy= -1.25543278
Zero-point correction (ZPE)= -568.3145 0.04226
Internal Energy (U)= -568.3105 0.04624
Enthalpy (H)= -568.3096 0.04718
Gibbs Free Energy (G)= -568.3423 0.01449

Frequencies -- 454.0770 533.7231 576.9224

Supporting Information: **34dichloroisothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1485.22235361 Predicted Change= -2.569976D-08
MP2 Energy= -1487.523394491 Correl. Energy= -2.30104088

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00020	0.00180	[YES]	0.00020	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.038695	0.702706	0.000023
C	0.132708	-0.731265	0.000033
C	-1.116844	-1.285173	0.000030
S	-2.287389	-0.022748	-0.000172
N	-1.159205	1.222899	-0.000060
Cl	1.428045	1.740785	0.000045
H	-1.375714	-2.335486	0.000070
Cl	1.616721	-1.621870	0.000108

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1485.22235361 Predicted Change= -2.569976D-08
MP2 Energy= -1487.523394491 MP2 Cor. Energy= -2.30104088
Zero-point correction (ZPE)= -1488.1874 0.03628
Internal Energy (U)= -1488.1812 0.04244
Enthalpy (H)= -1488.1803 0.04338
Gibbs Free Energy (G)= -1488.2190 0.00462

Frequencies -- 177.7101 178.3086 255.6405

Supporting Information: **3chloro4radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64609812 Predicted Change= -1.049428D-07
MP2 Energy= -1027.38218529 Correl. Energy= -1.73608717

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.557715	0.064881	0.000001
C	-0.147020	1.294009	0.000084
C	-1.490179	1.152512	0.000023
S	-1.806651	-0.561317	-0.000059
N	-0.179399	-1.018193	-0.000098
Cl	2.289094	-0.050371	0.000054
H	-2.275489	1.896322	0.000059

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64609812 Predicted Change= -1.049428D-07
MP2 Energy= -1027.38218529 MP2 Cor. Energy= -1.73608717
Zero-point correction (ZPE)= -1027.9064 0.03312
Internal Energy (U)= -1027.9015 0.03808
Enthalpy (H)= -1027.9005 0.03903
Gibbs Free Energy (G)= -1027.9365 0.00304

Frequencies -- 218.5079 301.5886 431.8266

Supporting Information: **45dichloroisothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1485.21654586 Predicted Change= -9.253061D-07
MP2 Energy= -1487.518781664 Correl. Energy= -2.3022358

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00121	0.00180	[YES]	0.00121	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.376870	-1.783480	0.000137
C	0.488280	-0.648857	-0.000119
C	-0.245508	0.512458	0.000049
S	-1.932511	0.112953	-0.000293
N	-1.669807	-1.548230	0.000429
Cl	2.215446	-0.752395	-0.000112
H	-0.025602	-2.811237	0.000445
Cl	0.339790	2.126564	0.000162

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1485.21654586 Predicted Change= -9.253061D-07
MP2 Energy= -1487.518781664 MP2 Cor. Energy= -2.3022358
Zero-point correction (ZPE)= -1488.1826 0.03655
Internal Energy (U)= -1488.1764 0.04276
Enthalpy (H)= -1488.1755 0.04370
Gibbs Free Energy (G)= -1488.2144 0.00479

Frequencies -- 165.1981 165.8131 256.7317

Supporting Information: **4chloro3radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64780634 Predicted Change= -3.536903D-07
MP2 Energy= -1027.389600622 Correl. Energy= -1.74179427

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00126	0.00180	[YES]	0.00126	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.162671	1.248559	-0.000104
C	-0.594997	0.039854	-0.000065
C	0.270066	-1.021622	0.000059
S	1.903774	-0.449080	0.000237
N	1.428556	1.222672	-0.000036
H	0.026491	-2.076424	0.000110
Cl	-2.324307	-0.052809	-0.000177

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64780634 Predicted Change= -3.536903D-07
MP2 Energy= -1027.389600622 MP2 Cor. Energy= -1.74179427
Zero-point correction (ZPE)= -1027.9127 0.03290
Internal Energy (U)= -1027.9077 0.03798
Enthalpy (H)= -1027.9067 0.03893
Gibbs Free Energy (G)= -1027.9429 0.00271

Frequencies -- 213.9297 283.0222 427.7408

Supporting Information: **4chloro5radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64179142 Predicted Change= -6.625751D-07
MP2 Energy= -1027.375649578 Correl. Energy= -1.73385815

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00028	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00131	0.00180	[YES]	0.00131	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.135718	1.208013	0.000425
C	-0.591546	-0.021360	0.000180
C	0.299169	-1.052326	-0.000526
S	1.910527	-0.517149	0.000252
N	1.452102	1.119952	-0.000675
Cl	-2.321952	-0.150885	-0.000013
H	-0.320012	2.193805	0.000442

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64179142 Predicted Change= -6.625751D-07
MP2 Energy= -1027.375649578 MP2 Cor. Energy= -1.73385815
Zero-point correction (ZPE)= -1027.9014 0.03342
Internal Energy (U)= -1027.8964 0.03842
Enthalpy (H)= -1027.8955 0.03936
Gibbs Free Energy (G)= -1027.9316 0.00323

Frequencies -- 202.1640 272.5643 427.7037

Supporting Information: **4chloroisothiazole2.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1026.29588464 Predicted Change= -5.501735D-07
MP2 Energy= -1028.10475817 Correl. Energy= -1.80887353

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00274	0.00180	[NO]	0.00274	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.140985	1.239043	0.000034
C	0.573781	0.002562	0.000018
C	-0.280757	-1.066442	0.000179
S	-1.894945	-0.468474	-0.000094
H	0.328369	2.218447	-0.000014
H	-0.033565	-2.119374	0.000259
N	-1.452436	1.154942	0.000086
Cl	2.310537	-0.102297	-0.000043

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1026.29588464 Predicted Change= -5.501735D-07
MP2 Energy= -1028.10475817 MP2 Cor. Energy= -1.80887353
Zero-point correction (ZPE)= -1028.5861 0.04584
Internal Energy (U)= -1028.5811 0.05085
Enthalpy (H)= -1028.5802 0.05180
Gibbs Free Energy (G)= -1028.6156 0.01632

Frequencies -- 216.0863 280.0528 429.0316

Supporting Information: **4radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -566.718399094 Predicted Change= -5.705486D-07
MP2 Energy= -567.9637709083 Correl. Energy= -1.24537181

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00140	0.00180	[YES]	0.00140	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.409636	-0.294527	-0.000075
C	-0.999834	1.061626	0.000069
C	0.340835	1.248066	0.000135
S	1.053463	-0.338215	-0.000096
H	-2.431658	-0.658105	-0.000024
H	0.923974	2.158947	0.000216
N	-0.419415	-1.168628	0.000082

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -566.718399094 Predicted Change= -5.705486D-07
MP2 Energy= -567.9637709083 MP2 Cor. Energy= -1.24537181
Zero-point correction (ZPE)= -568.3043 0.04261
Internal Energy (U)= -568.3004 0.04649
Enthalpy (H)= -568.2995 0.04744
Gibbs Free Energy (G)= -568.3320 0.01490

Frequencies -- 460.3111 571.6772 620.3650

Supporting Information: **5chloro3radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64751259 Predicted Change= -9.074789D-07
MP2 Energy= -1027.391446952 Correl. Energy= -1.74393436

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00165	0.00180	[YES]	0.00165	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.660558	1.130259	-0.000180
C	0.268212	1.420556	0.000652
C	-0.386951	0.215967	-0.000265
S	0.735399	-1.120496	0.000404
H	-0.194966	2.396961	0.001174
N	2.109825	-0.055528	-0.000781
Cl	-2.093595	-0.040060	-0.000201

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64751259 Predicted Change= -9.074789D-07
MP2 Energy= -1027.391446952 MP2 Cor. Energy= -1.74393436
Zero-point correction (ZPE)= -1027.9135 0.03293
Internal Energy (U)= -1027.9084 0.03804
Enthalpy (H)= -1027.9075 0.03898
Gibbs Free Energy (G)= -1027.9437 0.00275

Frequencies -- 221.8919 255.5563 428.0570

Supporting Information: **5chloro4radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64020282 Predicted Change= -1.220253D-06
MP2 Energy= -1027.372443173 Correl. Energy= -1.73224035

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00040 ‖	0.00045	[YES]	0.00013 ‖	0.00030	[YES]
Displ	0.00134 ‖	0.00180	[YES]	0.00134 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.716301	1.091768	0.000316
C	-0.326501	1.347917	0.000159
C	0.441964	0.232820	-0.000227
S	-0.641504	-1.135789	0.000190
N	-2.043340	-0.188845	0.000064
H	-2.506690	1.834612	0.000425
Cl	2.157598	0.095582	-0.000318

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64020282 Predicted Change= -1.220253D-06
MP2 Energy= -1027.372443173 MP2 Cor. Energy= -1.73224035
Zero-point correction (ZPE)= -1027.9009 0.03343
Internal Energy (U)= -1027.8959 0.03843
Enthalpy (H)= -1027.8949 0.03938
Gibbs Free Energy (G)= -1027.9310 0.00327

Frequencies -- 212.4681 251.6502 433.5557

Supporting Information: **5chloroisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=restart
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1026.29321676 Predicted Change= -5.332559D-07
MP2 Energy= -1028.103184986 Correl. Energy= -1.80996822

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00027	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00257	0.00180	[NO]	0.00257	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.693700	1.042986	0.000123
C	0.304470	1.355584	0.000012
C	-0.423397	0.194953	-0.000027
S	0.646544	-1.170050	0.000082
H	2.488537	1.784510	0.000122
H	-0.119150	2.351902	0.000048
N	2.038200	-0.229946	-0.000241
Cl	-2.142949	0.037228	-0.000026

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1026.29321676 Predicted Change= -5.332559D-07
MP2 Energy= -1028.103184986 MP2 Cor. Energy= -1.80996822
Zero-point correction (ZPE)= -1028.5838 0.04595
Internal Energy (U)= -1028.5788 0.05096
Enthalpy (H)= -1028.5778 0.05191
Gibbs Free Energy (G)= -1028.6133 0.01643

Frequencies -- 221.8904 254.9597 439.0508

Supporting Information: **5radicalisothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -566.717786736 Predicted Change= -8.079051D-07
MP2 Energy= -567.9651799801 Correl. Energy= -1.24739324

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00143	0.00180	[YES]	0.00143	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.151830	0.722220	-0.000445
C	-1.311922	-0.697787	-0.000153
C	-0.064635	-1.246648	0.000666
S	1.178709	-0.083753	-0.000315
H	-1.972704	1.435273	-0.000583
H	-2.253534	-1.231847	-0.000157
N	0.076745	1.209988	0.000766

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -566.717786736 Predicted Change= -8.079051D-07
MP2 Energy= -567.9651799801 MP2 Cor. Energy= -1.24739324
Zero-point correction (ZPE)= -568.3029 0.04268
Internal Energy (U)= -568.2990 0.04656
Enthalpy (H)= -568.2981 0.04751
Gibbs Free Energy (G)= -568.3306 0.01496

Frequencies -- 434.7143 586.1959 612.0214

Chloroisoxazoles

Supporting Information: **3chloroisoxazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -703.592585086 Predicted Change= -1.883694D-07
MP2 Energy= -705.2048586916 Correl. Energy= -1.6122736

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00016	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00077	0.00180	[YES]	0.00077	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.846532	0.591647	0.000019
C	-0.609007	1.150837	0.000027
C	0.240395	0.008186	-0.000033
H	-2.848566	0.996867	-0.000022
H	-0.326345	2.191586	0.000003
N	-0.413497	-1.129232	0.000234
O	-1.758685	-0.752195	-0.000059
Cl	1.966455	0.013512	-0.000073

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -703.592585086 Predicted Change= -1.883694D-07
MP2 Energy= -705.2048586916 MP2 Cor. Energy= -1.6122736
Zero-point correction (ZPE)= -705.5766 0.04869
Internal Energy (U)= -705.5720 0.05328
Enthalpy (H)= -705.5710 0.05423
Gibbs Free Energy (G)= -705.6052 0.02008

Frequencies -- 258.8083 313.7285 488.2308

Supporting Information: **3radicalisoxazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -244.012408866 Predicted Change= -2.498017D-07
MP2 Energy= -245.0720692209 Correl. Energy= -1.05966035

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00105	0.00180	[YES]	0.00105	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.753450	0.761281	0.000201
C	1.081216	-0.560891	-0.000095
C	-0.210770	-1.152910	0.000207
H	1.346199	1.666280	0.000181
H	2.052369	-1.028508	-0.000197
N	-1.211592	-0.355432	0.000330
O	-0.582600	0.945671	-0.000521

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -244.012408866 Predicted Change= -2.498017D-07
MP2 Energy= -245.0720692209 MP2 Cor. Energy= -1.05966035
Zero-point correction (ZPE)= -245.2948 0.04479
Internal Energy (U)= -245.2911 0.04843
Enthalpy (H)= -245.2902 0.04937
Gibbs Free Energy (G)= -245.3216 0.01799

Frequencies -- 575.2077 596.2398 696.0390

Supporting Information: **4chloroisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcycle=1000 qcisd=maxcycle=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -703.588991916 Predicted Change= -4.765970D-07
MP2 Energy= -705.2015505137 Correl. Energy= -1.61255859

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00165	0.00180	[YES]	0.00165	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.564467	-1.086091	0.000371
C	-0.270216	-0.010807	-0.000002
C	0.608486	1.108605	0.000036
O	1.839700	-0.663289	-0.000651
H	0.401553	-2.153591	0.000403
H	0.356771	2.161081	0.000053
N	1.865510	0.736408	0.000838
Cl	-1.997113	0.004336	-0.000208

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -703.588991916 Predicted Change= -4.765970D-07
MP2 Energy= -705.2015505137 MP2 Cor. Energy= -1.61255859
Zero-point correction (ZPE)= -705.5741 0.04879
Internal Energy (U)= -705.5695 0.05341
Enthalpy (H)= -705.5686 0.05435
Gibbs Free Energy (G)= -705.6028 0.02009

Frequencies -- 255.9766 290.1499 482.6895

Supporting Information: **4radicalisoxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcycle=8000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -244.007733483 Predicted Change= -4.001078D-07
MP2 Energy= -245.0579830589 Correl. Energy= -1.05024957

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00092	0.00180	[YES]	0.00092	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.097743	0.394624	0.000051
C	0.026710	1.222180	-0.000125
C	-1.114272	0.388108	0.000122
O	0.652078	-0.881844	0.000035
H	2.168337	0.532002	-0.000001
H	-2.165187	0.643557	0.000036
N	-0.754408	-0.878611	-0.000087

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -244.007733483 Predicted Change= -4.001078D-07
MP2 Energy= -245.0579830589 MP2 Cor. Energy= -1.05024957
Zero-point correction (ZPE)= -245.2875 0.04549
Internal Energy (U)= -245.2840 0.04904
Enthalpy (H)= -245.2830 0.04999
Gibbs Free Energy (G)= -245.3143 0.01873

Frequencies -- 546.0150 630.2116 818.6892

Supporting Information: **5chloroisoxazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -703.591802169 Predicted Change= -6.559508D-08
MP2 Energy= -705.2048169273 Correl. Energy= -1.61301475

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00037	0.00180	[YES]	0.00037	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.233558	0.097069	-0.000012
C	0.617847	1.159969	-0.000078
C	1.890486	0.528082	0.000113
H	0.374835	2.210633	-0.000133
N	1.811727	-0.783135	-0.000136
H	2.870458	0.989373	0.000173
O	0.434178	-1.065753	0.000096
Cl	-1.944086	0.005720	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -703.591802169 Predicted Change= -6.559508D-08
MP2 Energy= -705.2048169273 MP2 Cor. Energy= -1.61301475
Zero-point correction (ZPE)= -705.5762 0.04867
Internal Energy (U)= -705.5716 0.05327
Enthalpy (H)= -705.5706 0.05422
Gibbs Free Energy (G)= -705.6048 0.02003

Frequencies -- 235.4615 309.7174 493.1686

Supporting Information: **5radicalisoxazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -244.009533093 Predicted Change= -9.874498D-08
MP2 Energy= -245.0703118514 Correl. Energy= -1.06077875

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ‖	0.00045	[YES]	0.00003 ‖	0.00030	[YES]
Displ	0.00051 ‖	0.00180	[YES]	0.00051 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.074115	-1.153480	0.000082
C	1.114815	-0.489867	0.000025
C	0.660736	0.860596	0.000009
H	2.118543	-0.881385	0.000042
N	-0.649407	0.983767	-0.000163
H	1.254691	1.767202	-0.000039
O	-1.129500	-0.384460	0.000055

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -244.009533093 Predicted Change= -9.874498D-08
MP2 Energy= -245.0703118514 MP2 Cor. Energy= -1.06077875
Zero-point correction (ZPE)= -245.2925 0.04492
Internal Energy (U)= -245.2888 0.04853
Enthalpy (H)= -245.2879 0.04948
Gibbs Free Energy (G)= -245.3193 0.01812

Frequencies -- 560.4896 626.3697 694.6342

Chloropyrazines

Supporting Information: 2chloropyrazine.out

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -721.691857790 Predicted Change= -1.936376D-07
MP2 Energy= -723.4563943229 Correl. Energy= -1.76453653

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00047	0.00180	[YES]	0.00047	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.459147	-0.031645	0.000021
C	0.228850	1.190478	-0.000010
N	1.560564	1.220515	0.000011
C	2.191359	0.038301	0.000048
C	1.490087	-1.166027	0.000054
N	0.150021	-1.202059	0.000042
H	-0.304781	2.137035	-0.000062
H	3.278446	0.056387	0.000081
H	2.005360	-2.123675	0.000098
Cl	-2.215295	-0.022681	-0.000068

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.691857790 Predicted Change= -1.936376D-07
MP2 Energy= -723.4563943229 MP2 Cor. Energy= -1.76453653
Zero-point correction (ZPE)= -723.8466 0.06733
Internal Energy (U)= -723.8413 0.07259
Enthalpy (H)= -723.8404 0.07354
Gibbs Free Energy (G)= -723.8763 0.03764

Frequencies -- 171.8386 306.4915 423.2542

Supporting Information: **2radicalpyrazine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=(maxcycle=1000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -262.112681481 Predicted Change= -7.204525D-07
MP2 Energy= -263.3426337473 Correl. Energy= -1.22995226

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00038	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00116	0.00180	[YES]	0.00116	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.369918	-1.316753	-0.000036
C	-1.344896	-0.311229	-0.000062
N	-0.954715	0.968218	-0.000022
C	0.362694	1.216058	0.000037
C	1.311843	0.194854	0.000062
N	0.898104	-1.087157	0.000017
H	-2.410605	-0.517485	-0.000063
H	0.667900	2.260003	0.000032
H	2.380645	0.392472	0.000062

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -262.112681481 Predicted Change= -7.204525D-07
MP2 Energy= -263.3426337473 MP2 Cor. Energy= -1.22995226
Zero-point correction (ZPE)= -263.5740 0.06411
Internal Energy (U)= -263.5699 0.06827
Enthalpy (H)= -263.5689 0.06921
Gibbs Free Energy (G)= -263.6019 0.03619

Frequencies -- 364.5275 433.1714 570.9275

Chloropyrazoles

Supporting Information: 3chloropyrazole.out

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -683.796104029 Predicted Change= -1.235731D-06
MP2 Energy= -685.3829639388 Correl. Energy= -1.58685991

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00030	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00161	0.00180	[YES]	0.00161	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.853146	0.650341	0.000047
C	0.571595	1.164890	0.000041
C	-0.249719	0.014971	0.000013
N	1.722541	-0.701450	-0.000012
H	2.453971	-1.396672	-0.000133
H	2.820903	1.131435	0.000107
H	0.265720	2.199483	0.000085
Cl	-1.983184	-0.009995	0.000003
N	0.437945	-1.119341	-0.000090

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.796104029 Predicted Change= -1.235731D-06
MP2 Energy= -685.3829639388 MP2 Cor. Energy= -1.58685991
Zero-point correction (ZPE)= -685.7300 0.06193
Internal Energy (U)= -685.7252 0.06672
Enthalpy (H)= -685.7243 0.06766
Gibbs Free Energy (G)= -685.7587 0.03324

Frequencies -- 254.6736 317.2278 481.5302

Supporting Information: **3radicalpyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -224.213405407 Predicted Change= -8.606087D-08
MP2 Energy= -225.254566439 Correl. Energy= -1.04116103

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.538165	0.954401	0.000079
C	-1.204299	-0.261355	0.000019
C	-0.140731	-1.188650	0.000066
N	0.794263	0.678631	-0.000055
H	1.567711	1.327097	-0.000147
H	-0.906770	1.971389	0.000136
H	-2.268536	-0.437118	0.000050
N	1.049562	-0.662594	-0.000091

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -224.213405407 Predicted Change= -8.606087D-08
MP2 Energy= -225.254566439 MP2 Cor. Energy= -1.04116103
Zero-point correction (ZPE)= -225.4449 0.05828
Internal Energy (U)= -225.4411 0.06208
Enthalpy (H)= -225.4401 0.06303
Gibbs Free Energy (G)= -225.4718 0.03139

Frequencies -- 424.3146 599.7774 651.6563

Supporting Information: **4chloropyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -683.792850662 Predicted Change= -9.154105D-08
MP2 Energy= -685.379990396 Correl. Energy= -1.58713973

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00126	0.00180	[YES]	0.00126	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.559978	-1.100793	0.000066
C	-0.276469	-0.001289	-0.000017
C	0.573503	1.126459	0.000094
N	1.817484	-0.588829	0.000092
H	2.688945	-1.097518	0.000191
H	0.354266	-2.160625	0.000063
N	1.853602	0.759873	0.000007
H	0.299430	2.172273	0.000110
Cl	-2.010724	-0.015159	-0.000113

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.792850662 Predicted Change= -9.154105D-08
MP2 Energy= -685.379990396 MP2 Cor. Energy= -1.58713973
Zero-point correction (ZPE)= -685.7276 0.06209
Internal Energy (U)= -685.7228 0.06690
Enthalpy (H)= -685.7219 0.06784
Gibbs Free Energy (G)= -685.7564 0.03332

Frequencies -- 249.3792 292.2446 480.3855

Supporting Information: **4radicalpyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -224.208357482 Predicted Change= -4.293281D-07
MP2 Energy= -225.2449907232 Correl. Energy= -1.03663324

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00115	0.00180	[YES]	0.00115	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.053073	-0.556141	0.000001
C	0.146882	-1.228103	0.000054
C	1.170527	-0.269441	0.000191
N	-0.700602	0.760132	0.000093
H	-1.304715	1.568990	0.000140
H	-2.081051	-0.885996	0.000022
N	0.637181	0.958976	-0.000348
H	2.243706	-0.394638	0.000149

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -224.208357482 Predicted Change= -4.293281D-07
MP2 Energy= -225.2449907232 MP2 Cor. Energy= -1.03663324
Zero-point correction (ZPE)= -225.4399 0.05875
Internal Energy (U)= -225.4361 0.06249
Enthalpy (H)= -225.4352 0.06344
Gibbs Free Energy (G)= -225.4667 0.03191

Frequencies -- 476.3810 564.2043 686.9909

Supporting Information: **5chloropyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3ClN2 C1[X(C3H3ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -683.793526860 Predicted Change= -1.090175D-07
MP2 Energy= -685.3810646405 Correl. Energy= -1.58753778

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00130	0.00180	[YES]	0.00130	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.244824	0.093077	-0.000002
C	0.618047	1.169414	-0.000069
C	1.897782	0.568551	0.000059
N	0.513090	-1.032602	0.000054
H	0.192237	-1.989766	0.000162
H	0.356737	2.216445	-0.000142
N	1.837228	-0.762888	0.000006
H	2.863439	1.056888	0.000087
Cl	-1.970039	0.017566	-0.000027

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -683.793526860 Predicted Change= -1.090175D-07
MP2 Energy= -685.3810646405 MP2 Cor. Energy= -1.58753778
Zero-point correction (ZPE)= -685.7279 0.06198
Internal Energy (U)= -685.7231 0.06680
Enthalpy (H)= -685.7221 0.06774
Gibbs Free Energy (G)= -685.7567 0.03322

Frequencies -- 236.7237 298.7106 473.9444

Supporting Information: **5radicalpyrazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H3N2(2) C1[X(C3H3N2)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -224.209750452 Predicted Change= -1.422639D-07
MP2 Energy= -225.2489081172 Correl. Energy= -1.03915766

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00072	0.00180	[YES]	0.00072	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.079121	-1.184030	0.000174
C	1.123996	-0.515213	0.000033
C	0.712377	0.840620	0.000160
N	-1.087192	-0.296976	0.000056
H	-2.081695	-0.461044	0.000056
H	2.121341	-0.925911	0.000099
N	-0.615474	0.984484	-0.000423
H	1.335503	1.726139	0.000213

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -224.209750452 Predicted Change= -1.422639D-07
MP2 Energy= -225.2489081172 MP2 Cor. Energy= -1.03915766
Zero-point correction (ZPE)= -225.4416 0.05843
Internal Energy (U)= -225.4378 0.06223
Enthalpy (H)= -225.4369 0.06318
Gibbs Free Energy (G)= -225.4685 0.03153

Frequencies -- 408.0836 572.3938 674.8813

Chlorpyridazines

Supporting Information: **3chloropyridazine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -721.657259938 Predicted Change= -7.062171D-08
MP2 Energy= -723.424972686 Correl. Energy= -1.76771274

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00056	0.00180	[YES]	0.00056	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.461187	-1.262737	-0.000004
C	2.175327	-0.136941	-0.000001
C	1.604469	1.142286	0.000003
C	0.224982	1.220754	0.000003
C	-0.456724	-0.003385	0.000000
N	0.124258	-1.193068	-0.000003
H	2.225512	2.033016	0.000006
H	3.252871	-0.277316	0.000000
H	-0.312684	2.162352	0.000006
Cl	-2.208949	-0.003747	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.657259938 Predicted Change= -7.062171D-08
MP2 Energy= -723.424972686 MP2 Cor. Energy= -1.76771274
Zero-point correction (ZPE)= -723.8160 0.06658
Internal Energy (U)= -723.8107 0.07190
Enthalpy (H)= -723.8098 0.07284
Gibbs Free Energy (G)= -723.8458 0.03687

Frequencies -- 178.1647 310.5459 383.5200

Supporting Information: **4chloropyridazine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -721.656165625 Predicted Change= -7.747159D-08
MP2 Energy= -723.4239366652 Correl. Energy= -1.76777104

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00052	0.00180	[YES]	0.00052	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.563762	-1.214018	-0.000002
C	-0.230386	-1.173927	-0.000003
C	0.490581	0.026011	0.000000
C	-0.223696	1.209443	0.000003
C	-1.617624	1.086111	0.000003
N	-2.267661	-0.080005	0.000000
H	0.276278	-2.134877	-0.000005
H	0.263449	2.178553	0.000005
H	-2.251657	1.969263	0.000005
Cl	2.236390	0.009376	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.656165625 Predicted Change= -7.747159D-08
MP2 Energy= -723.4239366652 MP2 Cor. Energy= -1.76777104
Zero-point correction (ZPE)= -723.8150 0.06675
Internal Energy (U)= -723.8097 0.07207
Enthalpy (H)= -723.8088 0.07301
Gibbs Free Energy (G)= -723.8448 0.03700

Frequencies -- 181.1366 291.2619 388.9733

Chloropyridines

Supporting Information: 23dichloropyridine.out

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=(restart,maxcyc=1000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3Cl2N C1[X(C5H3Cl2N)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -1164.62403295 Predicted Change= -4.042971D-07
MP2 Energy= -1166.844069177 Correl. Energy= -2.22003622

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00028	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00090	0.00180	[YES]	0.00090	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.011953	-0.702001	-0.000067
C	-0.022909	0.703617	0.000027
C	1.191838	1.386592	0.000241
C	2.379571	0.657487	0.000364
C	2.299524	-0.732526	0.000285
N	1.136139	-1.394198	0.000069
H	1.194984	2.471539	0.000308
H	3.341448	1.160009	0.000523
H	3.195283	-1.348790	0.000365
Cl	-1.475731	-1.628194	-0.000286
Cl	-1.515125	1.604524	-0.000113

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1164.62403295 Predicted Change= -4.042971D-07
MP2 Energy= -1166.844069177 MP2 Cor. Energy= -2.22003622
Zero-point correction (ZPE)= -1167.4031 0.06970
Internal Energy (U)= -1167.3966 0.07621
Enthalpy (H)= -1167.3956 0.07716
Gibbs Free Energy (G)= -1167.4349 0.03784

Frequencies -- 124.0849 201.8844 248.5363

Supporting Information: **24dichloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=(restart,maxcyc=1000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3Cl2N C1[X(C5H3Cl2N)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -1164.62995437 Predicted Change= -2.009001D-07
MP2 Energy= -1166.84697145 Correl. Energy= -2.21701707

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00111	0.00180	[YES]	0.00111	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.178687	0.025308	-0.000113
C	-0.002263	-0.723339	-0.000056
C	-1.191814	-0.002337	0.000147
C	-1.167679	1.392715	0.000264
C	0.080907	2.009404	0.000145
N	1.245036	1.344086	-0.000030
H	0.012189	-1.805622	-0.000158
H	-2.082683	1.973221	0.000433
H	0.154920	3.094432	0.000247
Cl	2.707991	-0.845586	-0.000416
Cl	-2.718974	-0.853305	0.000261

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1164.62995437 Predicted Change= -2.009001D-07
MP2 Energy= -1166.84697145 MP2 Cor. Energy= -2.21701707
Zero-point correction (ZPE)= -1167.4075 0.06969
Internal Energy (U)= -1167.4010 0.07621
Enthalpy (H)= -1167.4000 0.07715
Gibbs Free Energy (G)= -1167.4394 0.03773

Frequencies -- 159.7764 202.4522 203.7458

Supporting Information: **2chloro3radicalpyridine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=10000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -705.057356241 Predicted Change= -6.811516D-07
MP2 Energy= -706.6911714717 Correl. Energy= -1.63381523

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00044	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00118	0.00180	[YES]	0.00118	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.497680	0.025523	0.000069
C	0.226377	1.199125	0.000050
C	1.600345	1.216993	0.000219
C	2.243448	-0.032494	0.000347
C	1.448286	-1.178160	0.000249
N	0.107948	-1.154404	0.000097
H	2.166716	2.144832	0.000256
H	3.326961	-0.108382	0.000491
H	1.899552	-2.167606	0.000319
Cl	-2.251383	0.048592	-0.000432

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.057356241 Predicted Change= -6.811516D-07
MP2 Energy= -706.6911714717 MP2 Cor. Energy= -1.63381523
Zero-point correction (ZPE)= -707.1269 0.06637
Internal Energy (U)= -707.1216 0.07171
Enthalpy (H)= -707.1206 0.07265
Gibbs Free Energy (G)= -707.1572 0.03604

Frequencies -- 179.7700 299.2747 418.8874

Supporting Information: **2chloro4radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -705.060084964 Predicted Change= -1.734965D-07
MP2 Energy= -706.6975548603 Correl. Energy= -1.63746989

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00021	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00075	0.00180	[YES]	0.00075	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.434892	0.006563	-0.000097
C	0.170357	1.278016	0.000014
C	1.542200	1.242111	0.000224
C	2.297625	0.090308	0.000340
C	1.555714	-1.099999	0.000250
N	0.217272	-1.140861	0.000030
H	-0.420854	2.186937	-0.000069
H	3.382696	0.077121	0.000503
H	2.062820	-2.063437	0.000330
Cl	-2.195976	-0.077446	-0.000315

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -705.060084964 Predicted Change= -1.734965D-07
MP2 Energy= -706.6975548603 MP2 Cor. Energy= -1.63746989
Zero-point correction (ZPE)= -707.1298 0.06612
Internal Energy (U)= -707.1244 0.07146
Enthalpy (H)= -707.1235 0.07240
Gibbs Free Energy (G)= -707.1601 0.03581

Frequencies -- 174.5523 315.2681 418.8293

Supporting Information: **2chloro5radicalpyridine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=10000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -705.058103922 Predicted Change= -1.170657D-06
MP2 Energy= -706.6915384347 Correl. Energy= -1.63343451

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00042	0.00045	[YES]	0.00011	0.00030	[YES]
Displ	0.00136	0.00180	[YES]	0.00136	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.406681	-0.013151	-0.000083
C	0.260303	1.217799	0.000013
C	1.659093	1.183706	0.000216
C	2.245496	-0.064313	0.000329
C	1.526386	-1.239707	0.000273
N	0.177791	-1.197982	0.000042
H	2.238218	2.103348	0.000283
H	-0.291245	2.151824	-0.000078
H	1.983928	-2.224804	0.000313
Cl	-2.169590	-0.008853	-0.000311

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -705.058103922 Predicted Change= -1.170657D-06
MP2 Energy= -706.6915384347 MP2 Cor. Energy= -1.63343451
Zero-point correction (ZPE)= -707.1267 0.06633
Internal Energy (U)= -707.1213 0.07167
Enthalpy (H)= -707.1204 0.07261
Gibbs Free Energy (G)= -707.1570 0.03603

Frequencies -- 191.2371 310.7208 408.3554

Supporting Information: **2chloropyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H4ClN C1[X(C5H4ClN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -705.702196576 Predicted Change= -8.884996D-07
MP2 Energy= -707.4275142555 Correl. Energy= -1.72531767

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00116	0.00180	[YES]	0.00116	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.469882	-0.015670	-0.000041
C	0.197185	1.212709	-0.000003
C	1.589174	1.179347	0.000220
C	2.240415	-0.055755	0.000319
C	1.460420	-1.210271	0.000194
N	0.119421	-1.196715	0.000063
H	2.154606	2.107117	0.000321
H	-0.355542	2.145012	-0.000132
H	3.323520	-0.124223	0.000480
H	1.922040	-2.195485	0.000329
Cl	-2.234379	-0.012798	-0.000328

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.702196576 Predicted Change= -8.884996D-07
MP2 Energy= -707.4275142555 MP2 Cor. Energy= -1.72531767
Zero-point correction (ZPE)= -707.8037 0.07936
Internal Energy (U)= -707.7984 0.08472
Enthalpy (H)= -707.7974 0.08567
Gibbs Free Energy (G)= -707.8334 0.04964

Frequencies -- 177.5455 312.0598 420.4117

Supporting Information: **2radicalpyridine2.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcycle=5000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H4N(2) C1[X(C5H4N)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -246.133047246 Predicted Change= -1.601620D-06
MP2 Energy= -247.284809885 Correl. Energy= -1.15176263

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00012	0.00030	[YES]
Displ	0.00164	0.00180	[YES]	0.00164	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.007294	-1.013574	-0.000032
C	0.234915	-1.357293	-0.000032
C	1.332838	-0.500419	-0.000032
C	1.027165	0.863029	0.000034
C	-0.313285	1.270691	0.000052
C	-1.312508	0.301454	-0.000019
H	1.825216	1.602245	0.000072
H	2.355661	-0.862052	-0.000032
H	-0.577275	2.323839	0.000119
H	-2.367292	0.566216	0.000040

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -246.133047246 Predicted Change= -1.601620D-06
MP2 Energy= -247.284809885 MP2 Cor. Energy= -1.15176263
Zero-point correction (ZPE)= -247.5300 0.07608
Internal Energy (U)= -247.5257 0.08034
Enthalpy (H)= -247.5248 0.08129
Gibbs Free Energy (G)= -247.5580 0.04810

Frequencies -- 387.4841 425.9593 574.5364

Supporting Information: **3chloro2radicalpyridine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=10000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -705.059133507 Predicted Change= -6.870792D-08
MP2 Energy= -706.6979595387 Correl. Energy= -1.63882603

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00030	0.00180	[YES]	0.00030	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.231904	-1.201464	-0.000125
C	-0.512174	-0.027411	-0.000048
C	0.206447	1.168201	0.000162
C	1.606317	1.113582	0.000284
C	2.239441	-0.125420	0.000193
N	1.514319	-1.263630	-0.000015
H	-0.316748	2.120287	0.000229
H	2.191675	2.027796	0.000448
H	3.321300	-0.223222	0.000278
Cl	-2.260475	-0.037905	-0.000214

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.059133507 Predicted Change= -6.870792D-08
MP2 Energy= -706.6979595387 MP2 Cor. Energy= -1.63882603
Zero-point correction (ZPE)= -707.1327 0.06656
Internal Energy (U)= -707.1273 0.07192
Enthalpy (H)= -707.1264 0.07286
Gibbs Free Energy (G)= -707.1630 0.03621

Frequencies -- 186.7384 290.9025 423.6865

Supporting Information: **3radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcycle=2000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H4N(2) C1[X(C5H4N)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -246.127995405 Predicted Change= -9.508303D-07
MP2 Energy= -247.2714976836 Correl. Energy= -1.14350227

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00044	0.00045	[YES]	0.00010	0.00030	[YES]
Displ	0.00072	0.00180	[YES]	0.00072	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.175635	0.734542	-0.000020
C	-1.270836	-0.609153	-0.000020
C	-0.124179	-1.378937	-0.000020
C	1.147419	-0.851772	0.000020
C	1.234086	0.548136	0.000040
C	0.045370	1.281948	-0.000003
H	2.039300	-1.473602	0.000035
H	-2.272049	-1.032440	-0.000083
H	2.196991	1.052760	0.000072
H	0.074048	2.370163	0.000011

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -246.127995405 Predicted Change= -9.508303D-07
MP2 Energy= -247.2714976836 MP2 Cor. Energy= -1.14350227
Zero-point correction (ZPE)= -247.5209 0.07596
Internal Energy (U)= -247.5166 0.08021
Enthalpy (H)= -247.5157 0.08116
Gibbs Free Energy (G)= -247.5489 0.04798

Frequencies -- 391.0957 423.5493 577.5448

Supporting Information: **4chloro2radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -705.061993900 Predicted Change= -8.889267D-08
MP2 Energy= -706.7026155491 Correl. Energy= -1.64062164

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00075	0.00180	[YES]	0.00075	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.565707	1.211922	0.000248
C	0.175719	1.273705	0.000186
C	-0.453388	0.028527	-0.000021
C	0.299220	-1.153429	-0.000136
C	1.685927	-1.047427	-0.000032
N	2.300284	0.154573	0.000151
H	-0.382737	2.202269	0.000274
H	-0.187257	-2.122002	-0.000302
H	2.319276	-1.930871	-0.000127
Cl	-2.205316	-0.065365	-0.000139

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.061993900 Predicted Change= -8.889267D-08
MP2 Energy= -706.7026155491 MP2 Cor. Energy= -1.64062164
Zero-point correction (ZPE)= -707.1348 0.06653
Internal Energy (U)= -707.1295 0.07189
Enthalpy (H)= -707.1285 0.07283
Gibbs Free Energy (G)= -707.1652 0.03620

Frequencies -- 186.0137 301.6287 401.2603

Supporting Information: **4chloropyridine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H4ClN C1[X(C5H4ClN)] #Atoms= 11
Charge = 0 Multiplicity = 1

SCF Energy= -705.700122575 Predicted Change= -8.246239D-07
MP2 Energy= -707.4253125748 Correl. Energy= -1.72519

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00169	0.00180	[YES]	0.00169	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.593546	-1.140396	0.000004
C	0.199016	-1.204472	-0.000001
C	-0.499760	0.000014	-0.000039
C	0.199028	1.204485	-0.000005
C	1.593559	1.140383	0.000021
N	2.294355	-0.000011	-0.000006
H	2.174603	-2.060773	0.000028
H	-0.318915	-2.157024	0.000008
H	-0.318850	2.157064	-0.000010
H	2.174633	2.060747	0.000004
Cl	-2.252017	-0.000001	0.000008

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.700122575 Predicted Change= -8.246239D-07
MP2 Energy= -707.4253125748 MP2 Cor. Energy= -1.72519
Zero-point correction (ZPE)= -707.8012 0.07946
Internal Energy (U)= -707.7958 0.08483
Enthalpy (H)= -707.7949 0.08577
Gibbs Free Energy (G)= -707.8309 0.04973

Frequencies -- 188.5894 298.7225 392.8766

Supporting Information: **4radicalpyridine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcycle=2000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H4N(2) C1[X(C5H4N)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -246.129629299 Predicted Change= -1.704605D-07
MP2 Energy= -247.2764335465 Correl. Energy= -1.14680424

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-0.000023	-1.348003	-0.000018
C	-1.144593	-0.658913	-0.000018
C	-1.213190	0.746234	-0.000018
C	0.000017	1.393941	0.000004
C	1.213209	0.746208	0.000025
C	1.144582	-0.658937	0.000022
H	-2.063197	-1.245073	-0.000034
H	-2.171361	1.257530	-0.000018
H	2.171392	1.257483	0.000042
H	2.063174	-1.245117	0.000038

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -246.129629299 Predicted Change= -1.704605D-07
MP2 Energy= -247.2764335465 MP2 Cor. Energy= -1.14680424
Zero-point correction (ZPE)= -247.5229 0.07575
Internal Energy (U)= -247.5187 0.08000
Enthalpy (H)= -247.5178 0.08094
Gibbs Free Energy (G)= -247.5509 0.04778

Frequencies -- 379.7107 446.0950 616.5239

Supporting Information: **5chloro2radicalpyridine.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=10000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C5H3ClN(2) C1[X(C5H3ClN)] #Atoms= 10
Charge = 0 Multiplicity = 2

SCF Energy= -705.060510699 Predicted Change= -1.030232D-07
MP2 Energy= -706.698686068 Correl. Energy= -1.63817536

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ‖	0.00045	[YES]	0.00003 ‖	0.00030	[YES]
Displ	0.00048 ‖	0.00180	[YES]	0.00048 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.240948	-0.131499	0.000320
C	1.688986	1.147672	0.000259
C	0.294567	1.204959	0.000054
C	-0.429146	0.005843	-0.000059
C	0.241127	-1.214929	0.000033
N	1.587722	-1.241659	0.000216
H	-0.229139	2.156341	-0.000018
H	2.294445	2.047530	0.000350
H	-0.293314	-2.160363	-0.000062
Cl	-2.182643	0.033873	-0.000319

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -705.060510699 Predicted Change= -1.030232D-07
MP2 Energy= -706.698686068 MP2 Cor. Energy= -1.63817536
Zero-point correction (ZPE)= -707.1326 0.06652
Internal Energy (U)= -707.1273 0.07188
Enthalpy (H)= -707.1263 0.07283
Gibbs Free Energy (G)= -707.1630 0.03619

Frequencies -- 203.0534 293.9929 395.3791

Chloropyrimidines

Supporting Information: **24dichloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=(restart)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2Cl2N2 C1[X(C4H2Cl2N2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -1180.63267580 Predicted Change= -3.336397D-07
MP2 Energy= -1182.882948464 Correl. Energy= -2.25027266

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00022	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00060	0.00180	[YES]	0.00060	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.118308	0.024822	0.000061
N	0.002373	-0.694172	0.000024
C	1.124896	0.006583	0.000009
C	1.158550	1.401818	0.000013
C	-0.085923	2.023735	0.000017
N	-1.242039	1.345077	0.000029
H	2.087600	1.957549	0.000004
H	-0.167263	3.108435	0.000006
Cl	-2.606131	-0.890948	-0.000048
Cl	2.622721	-0.895174	-0.000010

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1180.63267580 Predicted Change= -3.336397D-07
MP2 Energy= -1182.882948464 MP2 Cor. Energy= -2.25027266
Zero-point correction (ZPE)= -1183.4583 0.05766
Internal Energy (U)= -1183.4520 0.06404
Enthalpy (H)= -1183.4510 0.06498
Gibbs Free Energy (G)= -1183.4902 0.02576

Frequencies -- 162.2530 174.6545 210.3685

Supporting Information: **25dichloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=(restart,maxcycle=10000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2Cl2N2 C1[X(C4H2Cl2N2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -1180.62728812 Predicted Change= -1.970353D-07
MP2 Energy= -1182.877615971 Correl. Energy= -2.25032785

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.307887	0.000000	0.000027
N	0.724385	-1.194343	0.000013
C	-0.611304	-1.190785	0.000002
C	-1.337437	0.000000	-0.000002
C	-0.611302	1.190785	0.000001
N	0.724385	1.194343	0.000010
H	-1.110381	-2.156893	0.000000
H	-1.110380	2.156893	-0.000006
Cl	3.055200	0.000000	-0.000007
Cl	-3.079182	0.000000	-0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1180.62728812 Predicted Change= -1.970353D-07
MP2 Energy= -1182.877615971 MP2 Cor. Energy= -2.25032785
Zero-point correction (ZPE)= -1183.4536 0.05770
Internal Energy (U)= -1183.4472 0.06412
Enthalpy (H)= -1183.4462 0.06507
Gibbs Free Energy (G)= -1183.4855 0.02577

Frequencies -- 88.7641 222.1060 311.4229

Supporting Information: **2chloro4radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=(restart,maxcyc=10000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClN2(2) C1[X(C4H2ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -721.061762534 Predicted Change= -2.481845D-08
MP2 Energy= -722.7453332521 Correl. Energy= -1.68357071

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00031	0.00180	[YES]	0.00031	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.427104	-0.011291	0.000034
N	-0.143002	-1.226299	0.000005
C	-1.433646	-1.254091	-0.000009
C	-2.258848	-0.135669	-0.000005
C	-1.556922	1.072157	-0.000003
N	-0.216535	1.142920	0.000013
H	-3.341233	-0.179502	-0.000013
H	-2.083731	2.025123	-0.000008
Cl	2.169153	0.041847	-0.000012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.061762534 Predicted Change= -2.481845D-08
MP2 Energy= -722.7453332521 MP2 Cor. Energy= -1.68357071
Zero-point correction (ZPE)= -723.1864 0.05447
Internal Energy (U)= -723.1812 0.05967
Enthalpy (H)= -723.1803 0.06062
Gibbs Free Energy (G)= -723.2167 0.02423

Frequencies -- 161.1892 329.9192 425.8177

Supporting Information: **2chloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -721.703149472 Predicted Change= -4.184238D-07
MP2 Energy= -723.4615366276 Correl. Energy= -1.75838715

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00028	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00090	0.00180	[YES]	0.00090	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.444394	-0.000001	0.000031
N	-0.133807	-1.196133	0.000012
C	-1.472848	-1.182728	-0.000002
C	-2.209087	0.000000	-0.000006
C	-1.472846	1.182729	-0.000002
N	-0.133806	1.196133	0.000009
H	-1.959362	-2.156189	-0.000003
H	-3.293364	0.000002	-0.000013
H	-1.959359	2.156190	-0.000010
Cl	2.196924	0.000000	-0.000014

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.703149472 Predicted Change= -4.184238D-07
MP2 Energy= -723.4615366276 MP2 Cor. Energy= -1.75838715
Zero-point correction (ZPE)= -723.8525 0.06742
Internal Energy (U)= -723.8472 0.07266
Enthalpy (H)= -723.8463 0.07360
Gibbs Free Energy (G)= -723.8821 0.03774

Frequencies -- 160.2917 329.6298 414.8918

Supporting Information: **2radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -262.132594337 Predicted Change= -7.242033D-08
MP2 Energy= -263.3215926432 Correl. Energy= -1.1889983

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00036	0.00180	[YES]	0.00036	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	-1.326549	-0.000014
N	1.193070	-0.785393	-0.000009
C	1.190745	0.561818	0.000004
C	0.000001	1.288489	0.000013
C	-1.190744	0.561819	0.000007
N	-1.193071	-0.785392	-0.000007
H	2.161262	1.054372	0.000009
H	0.000001	2.373293	0.000025
H	-2.161261	1.054373	0.000014

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -262.132594337 Predicted Change= -7.242033D-08
MP2 Energy= -263.3215926432 MP2 Cor. Energy= -1.1889983
Zero-point correction (ZPE)= -263.5779 0.06407
Internal Energy (U)= -263.5738 0.06825
Enthalpy (H)= -263.5728 0.06919
Gibbs Free Energy (G)= -263.6059 0.03614

Frequencies -- 379.6520 383.2446 586.1610

Supporting Information: **4chloro2radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=(restart,maxcyc=10000)
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClN2(2) C1[X(C4H2ClN2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -721.062100302 Predicted Change= -5.106616D-07
MP2 Energy= -722.7438229009 Correl. Energy= -1.68172259

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00029	0.00045	[YES]	0.00008	0.00030	[YES]
Displ	0.00095	0.00180	[YES]	0.00095	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.443584	-1.210243	0.000024
N	-0.130468	-1.237403	0.000015
C	0.437188	-0.033510	0.000001
C	-0.308573	1.149475	-0.000009
C	-1.693442	1.003826	0.000004
N	-2.282816	-0.210052	0.000021
H	0.167378	2.122190	-0.000024
H	-2.350100	1.871118	0.000000
Cl	2.183893	0.040094	-0.000021

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.062100302 Predicted Change= -5.106616D-07
MP2 Energy= -722.7438229009 MP2 Cor. Energy= -1.68172259
Zero-point correction (ZPE)= -723.1843 0.05447
Internal Energy (U)= -723.1791 0.05969
Enthalpy (H)= -723.1781 0.06064
Gibbs Free Energy (G)= -723.2146 0.02419

Frequencies -- 170.8870 315.7788 390.9529

Supporting Information: **4chloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -721.704519565 Predicted Change= -2.859635D-07
MP2 Energy= -723.4632033371 Correl. Energy= -1.75868377

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.480500	-1.149822	0.000008
N	-0.140267	-1.186014	0.000002
C	0.464525	-0.011134	0.000008
C	-0.218781	1.205572	0.000004
C	-1.607287	1.108579	0.000005
N	-2.255786	-0.064769	0.000008
H	-1.983451	-2.114078	0.000001
H	0.297826	2.157773	0.000002
H	-2.223847	2.005516	0.000009
Cl	2.219653	-0.012524	-0.000014

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.704519565 Predicted Change= -2.859635D-07
MP2 Energy= -723.4632033371 MP2 Cor. Energy= -1.75868377
Zero-point correction (ZPE)= -723.8538 0.06762
Internal Energy (U)= -723.8486 0.07286
Enthalpy (H)= -723.8476 0.07381
Gibbs Free Energy (G)= -723.8835 0.03793

Frequencies -- 172.3190 314.1974 384.2932

Supporting Information: **4radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=10000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -262.133782640 Predicted Change= -2.747307D-07
MP2 Energy= -263.3243232399 Correl. Energy= -1.1905406

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.244965	0.378573	-0.000021
N	1.030909	-0.954923	0.000006
C	-0.196072	-1.354065	0.000008
C	-1.303860	-0.513427	0.000001
C	-0.978320	0.845797	0.000005
N	0.285433	1.297603	-0.000003
H	2.276970	0.719779	0.000016
H	-2.330117	-0.862989	0.000000
H	-1.761525	1.603180	0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -262.133782640 Predicted Change= -2.747307D-07
MP2 Energy= -263.3243232399 MP2 Cor. Energy= -1.1905406
Zero-point correction (ZPE)= -263.5818 0.06427
Internal Energy (U)= -263.5777 0.06843
Enthalpy (H)= -263.5767 0.06937
Gibbs Free Energy (G)= -263.6097 0.03635

Frequencies -- 349.6074 435.7243 602.1446

Supporting Information: **5chloropyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN2 C1[X(C4H3ClN2)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -721.699107371 Predicted Change= -7.402033D-08
MP2 Energy= -723.4581703771 Correl. Energy= -1.759063

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00053	0.00180	[YES]	0.00053	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.173564	-0.000001	-0.000004
N	-1.577300	-1.196708	-0.000002
C	-0.241170	-1.192972	0.000000
C	0.480926	0.000000	0.000002
C	-0.241171	1.192973	0.000004
N	-1.577300	1.196709	0.000000
H	0.265663	-2.155620	-0.000002
H	-3.261076	0.000000	0.000000
H	0.265663	2.155620	0.000002
Cl	2.227166	0.000000	0.000000

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -721.699107371 Predicted Change= -7.402033D-08
MP2 Energy= -723.4581703771 MP2 Cor. Energy= -1.759063
Zero-point correction (ZPE)= -723.8492 0.06765
Internal Energy (U)= -723.8439 0.07293
Enthalpy (H)= -723.8429 0.07388
Gibbs Free Energy (G)= -723.8789 0.03794

Frequencies -- 186.2102 286.8819 418.8264

Supporting Information: **5radicalpyrimidine.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3N2(2) C1[X(C4H3N2)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -262.126702463 Predicted Change= -1.749339D-07
MP2 Energy= -263.3056514247 Correl. Energy= -1.17894896

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00006	0.00030	[YES]
Displ	0.00089	0.00180	[YES]	0.00089	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	1.240526	0.000006
N	-1.200979	0.653719	-0.000002
C	-1.201980	-0.694200	-0.000003
C	0.000000	-1.368857	0.000001
C	1.201980	-0.694200	-0.000004
N	1.200979	0.653719	0.000001
H	-2.169736	-1.190232	0.000000
H	0.000000	2.328786	-0.000005
H	2.169736	-1.190233	0.000007

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -262.126702463 Predicted Change= -1.749339D-07
MP2 Energy= -263.3056514247 MP2 Cor. Energy= -1.17894896
Zero-point correction (ZPE)= -263.5699 0.06430
Internal Energy (U)= -263.5657 0.06846
Enthalpy (H)= -263.5648 0.06940
Gibbs Free Energy (G)= -263.5978 0.03637

Frequencies -- 381.6012 399.0825 567.7609

Chloropyrroles

Supporting Information: **23dichloropyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3Cl2N C1[X(C4H3Cl2N)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -1126.73201128 Predicted Change= -2.039141D-07
MP2 Energy= -1128.769135076 Correl. Energy= -2.03712379

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00099	0.00180	[YES]	0.00099	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.466819	2.228235	0.000101
C	-0.809431	1.712991	0.000173
C	-0.686247	0.294899	0.000011
C	0.659188	-0.007178	-0.000006
N	1.354008	1.176444	0.000032
H	2.360596	1.243097	-0.000109
H	0.816721	3.249778	0.000140
H	-1.734243	2.271245	0.000280
Cl	1.473508	-1.524393	-0.000103
Cl	-1.985456	-0.850485	-0.000026

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1126.73201128 Predicted Change= -2.039141D-07
MP2 Energy= -1128.769135076 MP2 Cor. Energy= -2.03712379
Zero-point correction (ZPE)= -1129.2864 0.06393
Internal Energy (U)= -1129.2801 0.07018
Enthalpy (H)= -1129.2792 0.07113
Gibbs Free Energy (G)= -1129.3176 0.03268

Frequencies -- 165.1609 195.1941 240.7336

Supporting Information: **24dichloropyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=5000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3Cl2N C1[X(C4H3Cl2N)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -1126.73325482 Predicted Change= -1.660836D-07
MP2 Energy= -1128.769041565 Correl. Energy= -2.03578674

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00085	0.00180	[YES]	0.00085	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.676313	1.350999	0.000155
C	-1.133136	0.053018	0.000083
C	-0.020579	-0.834322	0.000108
C	1.092999	-0.026356	-0.000077
N	0.700430	1.286312	0.000022
H	1.330301	2.074374	-0.000073
H	-1.205956	2.290656	0.000237
Cl	2.771613	-0.440347	-0.000268
H	-0.040527	-1.913308	0.000148
Cl	-2.804827	-0.425296	0.000146

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1126.73325482 Predicted Change= -1.660836D-07
MP2 Energy= -1128.769041565 MP2 Cor. Energy= -2.03578674
Zero-point correction (ZPE)= -1129.2878 0.06380
Internal Energy (U)= -1129.2815 0.07008
Enthalpy (H)= -1129.2805 0.07103
Gibbs Free Energy (G)= -1129.3190 0.03253

Frequencies -- 147.9607 198.4095 277.2600

Supporting Information: **2chloro3radicalpyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN(2) C1[X(C4H3ClN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -667.148572026 Predicted Change= -2.734114D-07
MP2 Energy= -668.6361531805 Correl. Energy= -1.48758115

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00138	0.00180	[YES]	0.00138	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.842212	0.652391	0.000140
C	-1.930882	-0.728599	0.000117
C	-0.596531	-1.191510	0.000087
C	0.264366	-0.131437	-0.000013
N	-0.511944	1.009380	-0.000031
H	-0.149752	1.951804	-0.000181
H	-2.616072	1.407002	0.000198
H	-2.839391	-1.313325	0.000188
Cl	1.989434	-0.042130	-0.000116

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -667.148572026 Predicted Change= -2.734114D-07
MP2 Energy= -668.6361531805 MP2 Cor. Energy= -1.48758115
Zero-point correction (ZPE)= -668.9986 0.06048
Internal Energy (U)= -668.9935 0.06561
Enthalpy (H)= -668.9925 0.06655
Gibbs Free Energy (G)= -669.0282 0.03088

Frequencies -- 196.3570 301.7503 381.4914

Supporting Information: **2chloro4radicalpyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN(2) C1[X(C4H3ClN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -667.149851155 Predicted Change= -5.608970D-07
MP2 Energy= -668.6385850692 Correl. Energy= -1.48873391

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00020	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00190	0.00180	[NO]	0.00190	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.931340	-0.608045	0.000120
C	1.903931	0.758430	0.000113
C	0.580471	1.250786	0.000068
C	-0.199711	0.109719	-0.000021
N	0.600857	-1.003032	0.000088
H	0.257709	-1.952748	0.000036
H	2.735551	-1.327136	0.000164
Cl	-1.924893	-0.060891	-0.000151
H	0.227737	2.270907	0.000065

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -667.149851155 Predicted Change= -5.608970D-07
MP2 Energy= -668.6385850692 MP2 Cor. Energy= -1.48873391
Zero-point correction (ZPE)= -669.0006 0.06038
Internal Energy (U)= -668.9955 0.06552
Enthalpy (H)= -668.9946 0.06646
Gibbs Free Energy (G)= -669.0302 0.03081

Frequencies -- 208.0421 303.5377 380.7264

Supporting Information: **2chloropyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H4ClN C1[X(C4H4ClN)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -667.806778526 Predicted Change= -1.160967D-07
MP2 Energy= -669.3529330346 Correl. Energy= -1.5461545

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00063	0.00180	[YES]	0.00063	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.832165	-0.713209	0.000063
C	1.913868	0.661372	0.000181
C	0.585035	1.180161	-0.000059
C	-0.255281	0.091625	-0.000002
N	0.497273	-1.054999	-0.000002
H	0.119062	-1.989941	-0.000157
H	2.598651	-1.474154	0.000105
H	2.826907	1.240876	0.000316
H	0.279328	2.216282	-0.000120
Cl	-1.985858	0.004249	-0.000072

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -667.806778526 Predicted Change= -1.160967D-07
MP2 Energy= -669.3529330346 MP2 Cor. Energy= -1.5461545
Zero-point correction (ZPE)= -669.6858 0.07325
Internal Energy (U)= -669.6807 0.07834
Enthalpy (H)= -669.6797 0.07929
Gibbs Free Energy (G)= -669.7147 0.04434

Frequencies -- 216.0730 301.1781 423.1330

Supporting Information: **2radicalpyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H4N(2) C1[X(C4H4N)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -208.222010948 Predicted Change= -3.258373D-07
MP2 Energy= -209.2230072961 Correl. Energy= -1.00099634

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00135	0.00180	[YES]	0.00135	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.689295	0.888307	0.000292
C	-0.686953	0.928207	-0.000087
C	-1.181272	-0.420438	0.000120
C	-0.059285	-1.204173	-0.000113
N	1.070103	-0.445440	-0.000205
H	2.016289	-0.792457	-0.000397
H	1.427335	1.677582	0.000534
H	-1.293411	1.824949	-0.000138
H	-2.211644	-0.743412	0.000167

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -208.222010948 Predicted Change= -3.258373D-07
MP2 Energy= -209.2230072961 MP2 Cor. Energy= -1.00099634
Zero-point correction (ZPE)= -209.3976 0.06920
Internal Energy (U)= -209.3933 0.07345
Enthalpy (H)= -209.3924 0.07439
Gibbs Free Energy (G)= -209.4248 0.04198

Frequencies -- 272.2405 443.9055 618.1263

Supporting Information: **3chloro2radicalpyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN(2) C1[X(C4H3ClN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -667.147861378 Predicted Change= -3.917708D-07
MP2 Energy= -668.63479321 Correl. Energy= -1.48693183

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00203	0.00180	[NO]	0.00203	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.859817	0.664361	0.000141
C	0.557961	1.112701	-0.000007
C	-0.293661	-0.038115	0.000025
C	0.537871	-1.125342	-0.000106
N	1.836283	-0.720428	-0.000130
H	2.640799	-1.328031	-0.000255
H	2.794869	1.205574	0.000287
H	0.227781	2.142340	0.000025
Cl	-2.028786	-0.038737	0.000031

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -667.147861378 Predicted Change= -3.917708D-07
MP2 Energy= -668.63479321 MP2 Cor. Energy= -1.48693183
Zero-point correction (ZPE)= -668.9983 0.05955
Internal Energy (U)= -668.9935 0.06431
Enthalpy (H)= -668.9926 0.06526
Gibbs Free Energy (G)= -669.0276 0.03025

Frequencies -- -124.5801 296.4147 311.4581

Supporting Information: **3chloropyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H4ClN C1[X(C4H4ClN)] #Atoms= 10
Charge = 0 Multiplicity = 1

SCF Energy= -667.807326280 Predicted Change= -1.282250D-07
MP2 Energy= -669.3529460909 Correl. Energy= -1.54561981

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00084	0.00180	[YES]	0.00084	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.845757	0.713331	0.000062
C	0.543611	1.165227	0.000129
C	-0.282219	0.008336	-0.000015
C	0.521097	-1.110679	-0.000006
N	1.820323	-0.660374	-0.000005
H	2.633879	-1.255822	-0.000155
H	2.779755	1.256031	0.000106
H	0.213751	2.193915	0.000221
H	0.272820	-2.160741	-0.000053
Cl	-2.024232	-0.004003	-0.000065

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -667.807326280 Predicted Change= -1.282250D-07
MP2 Energy= -669.3529460909 MP2 Cor. Energy= -1.54561981
Zero-point correction (ZPE)= -669.6865 0.07335
Internal Energy (U)= -669.6814 0.07842
Enthalpy (H)= -669.6805 0.07936
Gibbs Free Energy (G)= -669.7154 0.04445

Frequencies -- 238.8483 295.2668 441.3609

Supporting Information: **3radicalpyrrole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H4N(2) C1[X(C4H4N)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -208.222652598 Predicted Change= -1.797223D-07
MP2 Energy= -209.2238587532 Correl. Energy= -1.00120615

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00118	0.00180	[YES]	0.00118	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.675833	0.885827	-0.000033
C	1.188218	-0.401000	-0.000070
C	0.056932	-1.245770	-0.000054
C	-1.100116	-0.514388	0.000083
N	-0.696885	0.810269	0.000047
H	-1.317532	1.605921	0.000161
H	1.179657	1.842587	-0.000054
H	2.233449	-0.675096	-0.000143
H	-2.142578	-0.793311	0.000146

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -208.222652598 Predicted Change= -1.797223D-07
MP2 Energy= -209.2238587532 MP2 Cor. Energy= -1.00120615
Zero-point correction (ZPE)= -209.3981 0.06976
Internal Energy (U)= -209.3941 0.07380
Enthalpy (H)= -209.3932 0.07475
Gibbs Free Energy (G)= -209.4252 0.04274

Frequencies -- 407.2522 537.5733 633.3533

Supporting Information: **4chloro2radicalpyrrole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClN(2) C1[X(C4H3ClN)] #Atoms= 9
Charge = 0 Multiplicity = 2

SCF Energy= -667.149588065 Predicted Change= -7.245162D-07
MP2 Energy= -668.6381116031 Correl. Energy= -1.48852353

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00024	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00241	0.00180	[NO]	0.00241	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.621677	-1.062746	-0.000075
C	-0.224649	0.022146	-0.000008
C	0.540022	1.234152	0.000044
C	1.837759	0.800739	0.000175
N	1.913088	-0.554968	0.000144
H	2.759613	-1.102688	0.000261
H	0.419145	-2.122750	-0.000198
H	0.164216	2.245269	0.000047
Cl	-1.963732	-0.064753	-0.000114

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -667.149588065 Predicted Change= -7.245162D-07
MP2 Energy= -668.6381116031 MP2 Cor. Energy= -1.48852353
Zero-point correction (ZPE)= -669.0007 0.05991
Internal Energy (U)= -668.9954 0.06525
Enthalpy (H)= -668.9944 0.06619
Gibbs Free Energy (G)= -669.0305 0.03014

Frequencies -- 211.5336 265.9687 297.4798

Chlorooxazoles

Supporting Information: **2chloro_oxazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -703.637770056 Predicted Change= -1.754474D-07
MP2 Energy= -705.2427814841 Correl. Energy= -1.60501142

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00084	0.00180	[YES]	0.00084	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.781309	-0.682708	0.000129
C	1.813516	0.671307	0.000114
C	-0.215390	0.101833	-0.000077
H	2.511624	-1.475422	0.000209
H	2.666275	1.334577	0.000188
N	0.511495	1.168277	0.000015
O	0.459971	-1.070651	0.000049
Cl	-1.924397	-0.000852	-0.000111

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -703.637770056 Predicted Change= -1.754474D-07
MP2 Energy= -705.2427814841 MP2 Cor. Energy= -1.60501142
Zero-point correction (ZPE)= -705.6103 0.04919
Internal Energy (U)= -705.6058 0.05375
Enthalpy (H)= -705.6048 0.05469
Gibbs Free Energy (G)= -705.6389 0.02062

Frequencies -- 235.6880 330.4828 506.9651

Supporting Information: **2radical_oxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -244.055689359 Predicted Change= -8.381489D-07
MP2 Energy= -245.1131518869 Correl. Energy= -1.05746252

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00014	0.00030	[YES]
Displ	0.00120	0.00180	[YES]	0.00120	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.689123	0.845006	0.000133
C	-0.664983	0.888378	0.000025
C	-0.111348	-1.129720	-0.000091
H	1.487564	1.569450	0.000235
H	-1.325119	1.743592	0.000075
N	-1.169288	-0.426488	0.000057
O	1.068228	-0.493702	-0.000139

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -244.055689359 Predicted Change= -8.381489D-07
MP2 Energy= -245.1131518869 MP2 Cor. Energy= -1.05746252
Zero-point correction (ZPE)= -245.3256 0.04559
Internal Energy (U)= -245.3221 0.04916
Enthalpy (H)= -245.3211 0.05011
Gibbs Free Energy (G)= -245.3524 0.01884

Frequencies -- 549.7043 607.9783 744.0671

Supporting Information: **4chloro_oxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -703.638244435 Predicted Change= -1.092722D-06
MP2 Energy= -705.2437210037 Correl. Energy= -1.60547656

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00041	0.00045	[YES]	0.00015	0.00030	[YES]
Displ	0.00130	0.00180	[YES]	0.00130	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.559319	1.102103	-0.000037
C	0.249676	0.010902	-0.000018
C	-1.724577	-0.711122	0.000072
H	-0.408639	2.168531	-0.000091
H	-2.639142	-1.285635	0.000165
N	-0.503742	-1.145457	0.000104
O	-1.848806	0.639155	0.000054
Cl	1.974691	-0.022896	-0.000079

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -703.638244435 Predicted Change= -1.092722D-06
MP2 Energy= -705.2437210037 MP2 Cor. Energy= -1.60547656
Zero-point correction (ZPE)= -705.6119 0.04932
Internal Energy (U)= -705.6073 0.05388
Enthalpy (H)= -705.6064 0.05483
Gibbs Free Energy (G)= -705.6405 0.02073

Frequencies -- 255.8151 317.1649 488.6537

Supporting Information: **4radical_oxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -244.055668760 Predicted Change= -3.429411D-07
MP2 Energy= -245.1105494011 Correl. Energy= -1.05488064

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013 ‖	0.00045	[YES]	0.00005 ‖	0.00030	[YES]
Displ	0.00121 ‖	0.00180	[YES]	0.00121 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.155140	0.170105	0.000199
C	-0.243000	1.168562	0.000075
C	0.867736	-0.596356	0.000500
H	-2.227519	0.081419	0.000172
H	1.626542	-1.365163	0.000456
N	1.023452	0.696460	-0.000140
O	-0.422595	-1.005668	-0.000537

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -244.055668760 Predicted Change= -3.429411D-07
MP2 Energy= -245.1105494011 MP2 Cor. Energy= -1.05488064
Zero-point correction (ZPE)= -245.3267 0.04603
Internal Energy (U)= -245.3231 0.04955
Enthalpy (H)= -245.3222 0.05049
Gibbs Free Energy (G)= -245.3534 0.01931

Frequencies -- 595.2682 657.6641 722.7893

Supporting Information: **5chloro_oxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNO C1[X(C3H2ClNO)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -703.636334756 Predicted Change= -9.468255D-07
MP2 Energy= -705.2422300837 Correl. Energy= -1.60589532

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00037	0.00045	[YES]	0.00014	0.00030	[YES]
Displ	0.00165	0.00180	[YES]	0.00165	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.241415	0.099157	-0.000023
C	0.625445	1.144259	0.000007
C	1.770199	-0.642525	0.000114
H	0.411982	2.202422	-0.000034
H	2.525176	-1.414820	0.000208
N	1.921332	0.642052	0.000102
O	0.473791	-1.063679	0.000061
Cl	-1.947187	-0.022229	-0.000116

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -703.636334756 Predicted Change= -9.468255D-07
MP2 Energy= -705.2422300837 MP2 Cor. Energy= -1.60589532
Zero-point correction (ZPE)= -705.6098 0.04932
Internal Energy (U)= -705.6053 0.05390
Enthalpy (H)= -705.6043 0.05484
Gibbs Free Energy (G)= -705.6385 0.02070

Frequencies -- 232.0297 309.9803 495.3910

Supporting Information: **5radical_oxazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NO(2) C1[X(C3H2NO)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -244.053412253 Predicted Change= -3.135072D-07
MP2 Energy= -245.1056409349 Correl. Energy= -1.05222868

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00019	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.316136	-1.127376	0.000098
C	1.188454	-0.090275	0.000079
C	-0.810280	0.675298	-0.000022
H	2.266363	-0.083149	0.000126
H	-1.714644	1.265457	-0.000104
N	0.421462	1.077612	-0.000102
O	-0.958476	-0.683935	-0.000029

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -244.053412253 Predicted Change= -3.135072D-07
MP2 Energy= -245.1056409349 MP2 Cor. Energy= -1.05222868
Zero-point correction (ZPE)= -245.3224 0.04578
Internal Energy (U)= -245.3189 0.04932
Enthalpy (H)= -245.3179 0.05026
Gibbs Free Energy (G)= -245.3492 0.01904

Frequencies -- 528.3367 663.3048 790.2237

Chlorothiazoles

Supporting Information: 24dichlorothiazole.out

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1485.22755157 Predicted Change= -2.616958D-07
MP2 Energy= -1487.525191342 Correl. Energy= -2.29763976

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00154	0.00180	[YES]	0.00154	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.899072	1.322739	0.000243
C	1.182142	-0.011710	0.000571
C	-0.983299	-0.207108	0.000851
H	1.583068	2.158749	-0.000111
N	0.121327	-0.879565	0.000401
S	-0.825075	1.537218	-0.000394
Cl	-2.547007	-0.940468	-0.000674
Cl	2.792969	-0.660756	0.000298

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1485.22755157 Predicted Change= -2.616958D-07
MP2 Energy= -1487.525191342 MP2 Cor. Energy= -2.29763976
Zero-point correction (ZPE)= -1488.1935 0.03627
Internal Energy (U)= -1488.1873 0.04246
Enthalpy (H)= -1488.1863 0.04341
Gibbs Free Energy (G)= -1488.2252 0.00454

Frequencies -- 169.7593 197.6051 243.7779

Supporting Information: **25dichlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1485.22242387 Predicted Change= -1.103800D-07
MP2 Energy= -1487.520366111 Correl. Energy= -2.29794224

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005 ‖	0.00045	[YES]	0.00002 ‖	0.00030	[YES]
Displ	0.00107 ‖	0.00180	[YES]	0.00107 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.215729	0.183970	0.000207
C	-0.633985	1.417870	0.000111
C	1.201665	0.215968	0.000661
H	-1.172662	2.357370	-0.000226
N	0.743329	1.422266	-0.000069
S	0.005684	-1.069939	0.000121
Cl	2.886985	-0.173369	-0.000237
Cl	-2.900708	-0.185517	-0.000180

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1485.22242387 Predicted Change= -1.103800D-07
MP2 Energy= -1487.520366111 MP2 Cor. Energy= -2.29794224
Zero-point correction (ZPE)= -1488.1892 0.03648
Internal Energy (U)= -1488.1829 0.04274
Enthalpy (H)= -1488.1820 0.04368
Gibbs Free Energy (G)= -1488.2210 0.00470

Frequencies -- 115.0769 194.3316 300.1956

Supporting Information: **2chloro4radicalthiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.65153359 Predicted Change= -9.103936D-08
MP2 Energy= -1027.389553829 Correl. Energy= -1.73802024

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00100	0.00180	[YES]	0.00100	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.066380	0.025188	0.000446
C	1.512790	1.257855	0.000041
C	-0.373279	0.229367	-0.000491
H	3.097523	-0.295213	0.000886
N	0.182462	1.406939	-0.000244
S	0.735140	-1.128822	-0.000170
Cl	-2.080726	-0.033334	0.000210

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.65153359 Predicted Change= -9.103936D-08
MP2 Energy= -1027.389553829 MP2 Cor. Energy= -1.73802024
Zero-point correction (ZPE)= -1027.9145 0.03311
Internal Energy (U)= -1027.9095 0.03812
Enthalpy (H)= -1027.9085 0.03906
Gibbs Free Energy (G)= -1027.9446 0.00301

Frequencies -- 219.7998 274.8980 447.5167

Supporting Information: **2chloro5radicalthiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64734344 Predicted Change= -1.407318D-07
MP2 Energy= -1027.382629523 Correl. Energy= -1.73528608

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00050	0.00180	[YES]	0.00050	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.016678	-0.172196	0.000014
C	-1.673283	1.136268	0.000372
C	0.338353	0.208084	-0.000153
H	-2.334914	1.992100	0.000428
N	-0.296265	1.334462	0.000174
S	-0.659792	-1.244354	0.000025
Cl	2.063240	0.090788	-0.000203

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64734344 Predicted Change= -1.407318D-07
MP2 Energy= -1027.382629523 MP2 Cor. Energy= -1.73528608
Zero-point correction (ZPE)= -1027.9077 0.03332
Internal Energy (U)= -1027.9027 0.03833
Enthalpy (H)= -1027.9018 0.03928
Gibbs Free Energy (G)= -1027.9379 0.00318

Frequencies -- 221.0438 271.8020 445.8031

Supporting Information: **2chlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1026.30167632 Predicted Change= -2.282916D-07
MP2 Energy= -1028.10810521 Correl. Energy= -1.80642888

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00116	0.00180	[YES]	0.00116	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.003482	-0.134251	0.000345
C	-1.578891	1.161560	-0.000472
C	0.394754	0.217656	-0.000280
H	-3.015202	-0.515862	0.000720
H	-2.228078	2.029280	-0.000502
N	-0.213294	1.356759	0.000406
S	-0.633650	-1.204009	-0.000075
Cl	2.117674	0.046096	0.000034

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1026.30167632 Predicted Change= -2.282916D-07
MP2 Energy= -1028.10810521 MP2 Cor. Energy= -1.80642888
Zero-point correction (ZPE)= -1028.5923 0.04590
Internal Energy (U)= -1028.5872 0.05091
Enthalpy (H)= -1028.5863 0.05186
Gibbs Free Energy (G)= -1028.6218 0.01641

Frequencies -- 220.5146 274.9304 446.6063

Supporting Information: **2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -566.728532799 Predicted Change= -3.454890D-07
MP2 Energy= -567.9822653753 Correl. Energy= -1.25373257

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00021 ‖	0.00045	[YES]	0.00006 ‖	0.00030	[YES]
Displ	0.00083 ‖	0.00180	[YES]	0.00083 ‖	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.071943	1.178247	-0.000014
C	-1.288884	0.566975	-0.000248
C	-0.052079	-1.249180	-0.000305
H	0.151630	2.236687	0.000290
H	-2.251294	1.063834	-0.000005
N	-1.237139	-0.826027	0.000340
S	1.202317	-0.030912	0.000046

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -566.728532799 Predicted Change= -3.454890D-07
MP2 Energy= -567.9822653753 MP2 Cor. Energy= -1.25373257
Zero-point correction (ZPE)= -568.3181 0.04263
Internal Energy (U)= -568.3141 0.04660
Enthalpy (H)= -568.3132 0.04755
Gibbs Free Energy (G)= -568.3459 0.01485

Frequencies -- 438.5656 551.9343 570.0781

Supporting Information: **45dichlorothiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HCl2NS C1[X(C3HCl2NS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1485.22215434 Predicted Change= -3.124820D-08
MP2 Energy= -1487.521629366 Correl. Energy= -2.29947502

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00017	0.00180	[YES]	0.00017	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.243577	0.503555	0.000028
C	0.466428	-0.669384	0.000052
C	-1.542684	-1.545656	0.000031
N	-0.271822	-1.819960	-0.000036
S	-1.952118	0.151433	-0.000012
Cl	2.193962	-0.767228	-0.000007
H	-2.320578	-2.300113	-0.000023
Cl	0.357581	2.113453	-0.000005

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1485.22215434 Predicted Change= -3.124820D-08
MP2 Energy= -1487.521629366 MP2 Cor. Energy= -2.29947502
Zero-point correction (ZPE)= -1488.1888 0.03651
Internal Energy (U)= -1488.1826 0.04270
Enthalpy (H)= -1488.1817 0.04365
Gibbs Free Energy (G)= -1488.2205 0.00478

Frequencies -- 156.3477 174.9657 255.6263

Supporting Information: **4chloro2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.65500254 Predicted Change= -3.959396D-08
MP2 Energy= -1027.39720608 Correl. Energy= -1.74220353

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00023	0.00180	[YES]	0.00023	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.337604	-1.012113	0.000121
C	-0.538511	0.032124	0.000127
C	1.288462	1.215210	0.000082
H	0.122483	-2.071109	0.000079
N	0.030090	1.295720	-0.000028
S	1.977069	-0.387595	-0.000069
Cl	-2.264209	-0.129926	-0.000044

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.65500254 Predicted Change= -3.959396D-08
MP2 Energy= -1027.39720608 MP2 Cor. Energy= -1.74220353
Zero-point correction (ZPE)= -1027.9191 0.03317
Internal Energy (U)= -1027.9141 0.03821
Enthalpy (H)= -1027.9131 0.03916
Gibbs Free Energy (G)= -1027.9493 0.00303

Frequencies -- 208.0239 300.0381 431.8788

Supporting Information: **4chloro5radicalthiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64755274 Predicted Change= -9.143191D-07
MP2 Energy= -1027.380315068 Correl. Energy= -1.73276232

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00043	0.00045	[YES]	0.00013	0.00030	[YES]
Displ	0.00133	0.00180	[YES]	0.00133	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.290926	-1.049445	0.000044
C	-0.581693	-0.012808	-0.000211
C	1.318134	1.111213	0.000094
N	0.019419	1.224640	-0.000074
S	1.933889	-0.531301	-0.000002
Cl	-2.307851	-0.136826	0.000047
H	1.991100	1.960625	0.000184

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64755274 Predicted Change= -9.143191D-07
MP2 Energy= -1027.380315068 MP2 Cor. Energy= -1.73276232
Zero-point correction (ZPE)= -1027.9063 0.03334
Internal Energy (U)= -1027.9013 0.03835
Enthalpy (H)= -1027.9003 0.03929
Gibbs Free Energy (G)= -1027.9365 0.00316

Frequencies -- 186.6087 293.4536 435.2187

Supporting Information: **4radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -566.726385406 Predicted Change= -9.780919D-08
MP2 Energy= -567.9742116424 Correl. Energy= -1.24782623

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00039	0.00180	[YES]	0.00039	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.195576	1.261923	0.000196
C	-1.113554	0.916081	0.000030
C	-0.389729	-1.120394	0.000001
H	0.677719	2.227700	0.000259
N	-1.465547	-0.372322	-0.000012
S	1.114256	-0.235178	-0.000094
H	-0.400751	-2.204263	-0.000028

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -566.726385406 Predicted Change= -9.780919D-08
MP2 Energy= -567.9742116424 MP2 Cor. Energy= -1.24782623
Zero-point correction (ZPE)= -568.3141 0.04256
Internal Energy (U)= -568.3102 0.04646
Enthalpy (H)= -568.3093 0.04741
Gibbs Free Energy (G)= -568.3418 0.01483

Frequencies -- 458.7138 596.3008 613.0396

Supporting Information: **5chloro2radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.65053307 Predicted Change= -5.856086D-08
MP2 Energy= -1027.39216893 Correl. Energy= -1.74163586

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00044	0.00180	[YES]	0.00044	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.367923	0.190757	-0.000076
C	-0.360682	1.343253	0.000097
C	-2.034702	-0.093791	-0.000175
H	0.038790	2.349109	0.000231
N	-1.734343	1.127927	0.000004
S	-0.698850	-1.219538	0.000069
Cl	2.085175	0.036865	-0.000026

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.65053307 Predicted Change= -5.856086D-08
MP2 Energy= -1027.39216893 MP2 Cor. Energy= -1.74163586
Zero-point correction (ZPE)= -1027.9165 0.03336
Internal Energy (U)= -1027.9114 0.03844
Enthalpy (H)= -1027.9104 0.03939
Gibbs Free Energy (G)= -1027.9467 0.00315

Frequencies -- 226.4584 254.4814 432.6347

Supporting Information: **5chloro4radicalthiazole.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3HClNS(2) C1[X(C3HClNS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -1025.64670899 Predicted Change= -1.108616D-07
MP2 Energy= -1027.38033859 Correl. Energy= -1.7336296

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00059	0.00180	[YES]	0.00059	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.434001	0.233275	-0.000370
C	0.334795	1.348727	-0.000058
C	1.997559	-0.043244	0.000175
N	1.659682	1.222651	0.000009
S	0.653721	-1.158320	-0.000056
H	3.020296	-0.402574	0.000498
Cl	-2.146337	0.067328	0.000109

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1025.64670899 Predicted Change= -1.108616D-07
MP2 Energy= -1027.38033859 MP2 Cor. Energy= -1.7336296
Zero-point correction (ZPE)= -1027.9092 0.03334
Internal Energy (U)= -1027.9042 0.03836
Enthalpy (H)= -1027.9033 0.03931
Gibbs Free Energy (G)= -1027.9394 0.00317

Frequencies -- 213.9936 256.8915 442.0250

Supporting Information: **5chlorothiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2ClNS C1[X(C3H2ClNS)] #Atoms= 8
Charge = 0 Multiplicity = 1

SCF Energy= -1026.29729251 Predicted Change= -1.497737D-07
MP2 Energy= -1028.103925566 Correl. Energy= -1.80663306

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00086	0.00180	[YES]	0.00086	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.414997	0.184201	0.000040
C	0.310317	1.342093	0.000217
C	1.992876	-0.081567	0.000388
H	-0.117104	2.337540	0.000123
N	1.675137	1.178960	-0.000311
S	0.646108	-1.200165	-0.000019
H	3.011507	-0.452399	0.000376
Cl	-2.134546	0.023319	-0.000112

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1026.29729251 Predicted Change= -1.497737D-07
MP2 Energy= -1028.103925566 MP2 Cor. Energy= -1.80663306
Zero-point correction (ZPE)= -1028.5886 0.04603
Internal Energy (U)= -1028.5836 0.05107
Enthalpy (H)= -1028.5827 0.05201
Gibbs Free Energy (G)= -1028.6182 0.01648

Frequencies -- 220.3272 258.0534 437.1280

Supporting Information: **5radicalthiazole.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C3H2NS(2) C1[X(C3H2NS)] #Atoms= 7
Charge = 0 Multiplicity = 2

SCF Energy= -566.721677526 Predicted Change= -1.399916D-07
MP2 Energy= -567.9661038013 Correl. Energy= -1.24442627

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00015	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.125118	-1.237281	-0.000063
C	-1.332679	-0.622443	0.000076
C	0.011513	1.152479	0.000139
H	-2.307343	-1.092305	-0.000124
N	-1.230946	0.761406	-0.000062
S	1.205404	-0.136696	-0.000031
H	0.315206	2.193068	0.000143

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -566.721677526 Predicted Change= -1.399916D-07
MP2 Energy= -567.9661038013 MP2 Cor. Energy= -1.24442627
Zero-point correction (ZPE)= -568.3064 0.04273
Internal Energy (U)= -568.3025 0.04664
Enthalpy (H)= -568.3016 0.04759
Gibbs Free Energy (G)= -568.3342 0.01497

Frequencies -- 416.6415 581.9989 591.3524

Chlorothiophenes

Supporting Information: **235trichlorothiophene.out**

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 #g3b3
 #N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
 #N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
 #N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge
---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C4HCl3S   C1[X(C4HCl3S)]  #Atoms= 9
 Charge = 0     Multiplicity = 1
---------------------------------------------------------------------
 SCF Energy= -1928.14301545     Predicted Change= -1.461893D-07
 MP2 Energy= -1930.895830481     Correl. Energy= -2.75281503
=====================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00013 ||  0.00045   [ YES ]      0.00004 ||  0.00030   [ YES ]
 Displ      0.00076 ||  0.00180   [ YES ]      0.00076 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic        Coordinates (Angstroms)
      Type      X          Y      Z
---------------------------------------------------------------------
      C        1.546562      0.169044     -0.000044
      C        0.674571      1.215961      0.000056
      C       -0.685710      0.771076      0.000058
      C       -0.813743     -0.591511     -0.000023
      S        0.746037     -1.383220      0.000161
      H        0.965839      2.258302      0.000059
      Cl      -2.264330     -1.517523     -0.000093
      Cl      -2.021805      1.878035      0.000070
      Cl       3.272458      0.256300     -0.000149
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -1928.14301545 Predicted Change= -1.461893D-07
 MP2 Energy=     -1930.895830481        MP2 Cor. Energy= -2.75281503
 Zero-point correction (ZPE)=         -1931.7325  0.03866
 Internal Energy (U)=                 -1931.7247  0.04638
 Enthalpy (H)=                        -1931.7238   0.04732
 Gibbs Free Energy (G)=               -1931.7665    0.00458
---------------------------------------------------------------------
 Frequencies --   115.2525              169.8338              171.3710
```

Supporting Information: **23dichlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2Cl2S C1[X(C4H2Cl2S)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1469.22150678 Predicted Change= -1.110649D-09
MP2 Energy= -1471.482402178 Correl. Energy= -2.2608954

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00011	0.00180	[YES]	0.00011	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.719616	-1.470573	0.000016
C	0.401923	-1.820846	0.000015
C	-0.463858	-0.682798	-0.000004
C	0.214821	0.507578	0.000005
S	1.940172	0.252978	0.000107
H	2.583269	-2.121622	0.000002
H	0.036351	-2.840498	-0.000012
Cl	-0.445831	2.098492	-0.000041
Cl	-2.195191	-0.821179	-0.000070

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1469.22150678 Predicted Change= -1.110649D-09
MP2 Energy= -1471.482402178 MP2 Cor. Energy= -2.2608954
Zero-point correction (ZPE)= -1472.1350 0.04815
Internal Energy (U)= -1472.1286 0.05457
Enthalpy (H)= -1472.1276 0.05551
Gibbs Free Energy (G)= -1472.1668 0.01630

Frequencies -- 158.6812 173.4121 239.1591

Supporting Information: **24dichlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2Cl2S C1[X(C4H2Cl2S)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1469.22304594 Predicted Change= -4.119261D-10
MP2 Energy= -1471.482220632 Correl. Energy= -2.25917469

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ‖	0.00045	[YES]	0.00000 ‖	0.00030	[YES]
Displ	0.00003 ‖	0.00180	[YES]	0.00003 ‖	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.916800	1.297318	0.000007
C	-1.239227	-0.028462	-0.000002
C	-0.115773	-0.912109	0.000002
C	1.055266	-0.211183	0.000000
S	0.807246	1.515228	-0.000003
H	-1.582537	2.148486	0.000013
H	-0.186273	-1.991969	0.000003
Cl	2.655367	-0.868418	0.000001
Cl	-2.881715	-0.618261	-0.000001

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1469.22304594 Predicted Change= -4.119261D-10
MP2 Energy= -1471.482220632 MP2 Cor. Energy= -2.25917469
Zero-point correction (ZPE)= -1472.1366 0.04805
Internal Energy (U)= -1472.1301 0.05448
Enthalpy (H)= -1472.1292 0.05542
Gibbs Free Energy (G)= -1472.1685 0.01613

Frequencies -- 158.9394 187.3103 244.5124

Supporting Information: **2chloro3radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1009.64609758 Predicted Change= -3.743368D-09
MP2 Energy= -1011.341990069 Correl. Energy= -1.69589248

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00010	0.00180	[YES]	0.00010	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.023968	-0.166733	0.000029
C	-1.725848	1.170562	-0.000023
C	-0.321743	1.357984	-0.000031
C	0.445469	0.249815	-0.000006
S	-0.599807	-1.170825	-0.000001
H	-3.001099	-0.633107	0.000065
H	-2.463069	1.964166	-0.000028
Cl	2.165742	0.101904	0.000010

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1009.64609758 Predicted Change= -3.743368D-09
MP2 Energy= -1011.341990069 MP2 Cor. Energy= -1.69589248
Zero-point correction (ZPE)= -1011.8532 0.04491
Internal Energy (U)= -1011.8480 0.05014
Enthalpy (H)= -1011.8470 0.05109
Gibbs Free Energy (G)= -1011.8835 0.01459

Frequencies -- 191.1143 254.1043 432.8525

Supporting Information: **2chloro4radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1009.64766342 Predicted Change= -1.165885D-07
MP2 Energy= -1011.34472146 Correl. Energy= -1.69705804

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00012	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00054	0.00180	[YES]	0.00054	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.098518	-0.044982	0.000032
C	1.643530	1.221697	0.000007
C	0.244014	1.437762	-0.000011
C	-0.392288	0.223927	0.000017
S	0.709732	-1.132541	-0.000061
H	3.102258	-0.445609	0.000040
H	-0.260372	2.395307	-0.000010
Cl	-2.103543	-0.050557	0.000040

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1009.64766342 Predicted Change= -1.165885D-07
MP2 Energy= -1011.34472146 MP2 Cor. Energy= -1.69705804
Zero-point correction (ZPE)= -1011.8559 0.04472
Internal Energy (U)= -1011.8506 0.04996
Enthalpy (H)= -1011.8497 0.05091
Gibbs Free Energy (G)= -1011.8862 0.01445

Frequencies -- 207.4305 260.7109 430.1883

Supporting Information: **2chlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClS C1[X(C4H3ClS)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1010.29637297 Predicted Change= -2.024341D-07
MP2 Energy= -1012.064966053 Correl. Energy= -1.76859308

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.00144	0.00180	[YES]	0.00144	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.021288	-0.204049	0.000078
C	-1.703945	1.124893	-0.000043
C	-0.295489	1.367784	0.000002
C	0.421625	0.204668	0.000013
S	-0.601420	-1.207547	-0.000032
H	-3.001259	-0.662113	0.000125
H	-2.447065	1.914896	-0.000077
H	0.162997	2.349556	-0.000017
Cl	2.147213	0.044626	0.000010

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1010.29637297 Predicted Change= -2.024341D-07
MP2 Energy= -1012.064966053 MP2 Cor. Energy= -1.76859308
Zero-point correction (ZPE)= -1012.5346 0.05756
Internal Energy (U)= -1012.5294 0.06277
Enthalpy (H)= -1012.5284 0.06372
Gibbs Free Energy (G)= -1012.5642 0.02792

Frequencies -- 210.0654 260.3533 434.7617

Supporting Information: **2radical35dichlorothiophene.out**

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4HCl2S(2) C1[X(C4HCl2S)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1468.57032663 Predicted Change= -6.608251D-08
MP2 Energy= -1470.757248311 Correl. Energy= -2.18692168

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.420973	-1.759700	0.000078
C	0.080682	-1.918906	0.000031
C	-0.553828	-0.621775	-0.000049
C	0.329342	0.425326	0.000128
S	1.998414	-0.142347	-0.000197
H	-0.464877	-2.853946	0.000072
Cl	-0.023527	2.110398	0.000219
Cl	-2.280753	-0.440878	-0.000104

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1468.57032663 Predicted Change= -6.608251D-08
MP2 Energy= -1470.757248311 MP2 Cor. Energy= -2.18692168
Zero-point correction (ZPE)= -1471.4518 0.03541
Internal Energy (U)= -1471.4453 0.04191
Enthalpy (H)= -1471.4444 0.04285
Gibbs Free Energy (G)= -1471.4844 0.00278

Frequencies -- 155.1115 173.7482 195.9047

Supporting Information: **2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3S(2) C1[X(C4H3S)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -550.721537665 Predicted Change= -5.264263D-07
MP2 Energy= -551.9295600698 Correl. Energy= -1.2080224

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00017	0.00045	[YES]	0.00007	0.00030	[YES]
Displ	0.00171	0.00180	[YES]	0.00171	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.042255	1.188659	0.000178
C	-1.238468	0.711277	-0.000025
C	-1.317436	-0.728277	0.000160
C	-0.068767	-1.253720	0.000180
S	1.216888	-0.111448	-0.000211
H	0.377785	2.217443	0.000234
H	-2.113116	1.354117	-0.000080
H	-2.240385	-1.296018	0.000257

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -550.721537665 Predicted Change= -5.264263D-07
MP2 Energy= -551.9295600698 MP2 Cor. Energy= -1.2080224
Zero-point correction (ZPE)= -552.2522 0.05407
Internal Energy (U)= -552.2480 0.05821
Enthalpy (H)= -552.2471 0.05915
Gibbs Free Energy (G)= -552.2801 0.02618

Frequencies -- 364.4340 515.7536 605.7443

Supporting Information: **3chloro2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1009.64753337 Predicted Change= -5.211523D-08
MP2 Energy= -1011.342710605 Correl. Energy= -1.69517723

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.444432	1.104816	0.000078
C	0.087351	1.251990	-0.000057
C	-0.604463	-0.010198	0.000047
C	0.272076	-1.042819	0.000041
S	1.925030	-0.580598	-0.000208
H	2.202282	1.877294	0.000129
H	-0.426246	2.206756	-0.000078
Cl	-2.339582	-0.153954	0.000155

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1009.64753337 Predicted Change= -5.211523D-08
MP2 Energy= -1011.342710605 MP2 Cor. Energy= -1.69517723
Zero-point correction (ZPE)= -1011.8521 0.04483
Internal Energy (U)= -1011.8469 0.05012
Enthalpy (H)= -1011.8459 0.05106
Gibbs Free Energy (G)= -1011.8826 0.01440

Frequencies -- 163.6146 276.1845 402.3759

Supporting Information: **3chlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

#g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3ClS C1[X(C4H3ClS)] #Atoms= 9
Charge = 0 Multiplicity = 1

SCF Energy= -1010.30089557 Predicted Change= -1.421990D-07
MP2 Energy= -1012.068449978 Correl. Energy= -1.7675544

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00003	0.00030	[YES]
Displ	0.00140	0.00180	[YES]	0.00140	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.444962	1.136062	0.000169
C	-0.088121	1.287865	-0.000107
C	0.583567	0.026563	0.000056
C	-0.253939	-1.052363	0.000109
S	-1.909540	-0.536785	-0.000082
H	-2.202276	1.908238	0.000237
H	0.425058	2.241814	-0.000223
H	0.006960	-2.100757	0.000152
Cl	2.326096	-0.108794	-0.000013

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1010.30089557 Predicted Change= -1.421990D-07
MP2 Energy= -1012.068449978 MP2 Cor. Energy= -1.7675544
Zero-point correction (ZPE)= -1012.5386 0.05752
Internal Energy (U)= -1012.5334 0.06272
Enthalpy (H)= -1012.5324 0.06366
Gibbs Free Energy (G)= -1012.5682 0.02789

Frequencies -- 210.5953 284.1955 423.3272

Supporting Information: **3radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H3S(2) C1[X(C4H3S)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -550.723724783 Predicted Change= -6.583170D-07
MP2 Energy= -551.9333149071 Correl. Energy= -1.20959012

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00025	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.00130	0.00180	[YES]	0.00130	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.439594	-1.131287	0.000269
C	-1.489189	-0.248745	-0.000068
C	-0.999037	1.081198	-0.000003
C	0.336834	1.260956	0.000274
S	1.101298	-0.323955	-0.000217
H	-0.476216	-2.213265	0.000430
H	-2.533323	-0.537113	-0.000140
H	0.934690	2.160933	0.000341

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -550.723724783 Predicted Change= -6.583170D-07
MP2 Energy= -551.9333149071 MP2 Cor. Energy= -1.20959012
Zero-point correction (ZPE)= -552.2567 0.05409
Internal Energy (U)= -552.2526 0.05819
Enthalpy (H)= -552.2517 0.05913
Gibbs Free Energy (G)= -552.2846 0.02625

Frequencies -- 435.4440 548.3127 598.6793

Supporting Information: **4chloro2radicalthiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3 scf=maxcyc=1000
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4H2ClS(2) C1[X(C4H2ClS)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1009.64917573 Predicted Change= -4.546694D-08
MP2 Energy= -1011.345858003 Correl. Energy= -1.69668227

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00067	0.00180	[YES]	0.00067	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.327340	-1.005594	0.000016
C	0.548776	0.041487	0.000001
C	-0.063530	1.346567	0.000006
C	-1.407154	1.191424	0.000009
S	-1.980690	-0.427798	-0.000011
H	-0.108562	-2.064282	0.000023
H	0.484249	2.279943	0.000009
Cl	2.282990	-0.165541	-0.000003

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1009.64917573 Predicted Change= -4.546694D-08
MP2 Energy= -1011.345858003 MP2 Cor. Energy= -1.69668227
Zero-point correction (ZPE)= -1011.8551 0.04473
Internal Energy (U)= -1011.8498 0.04999
Enthalpy (H)= -1011.8489 0.05093
Gibbs Free Energy (G)= -1011.8854 0.01441

Frequencies -- 202.4091 285.1962 360.1925

Supporting Information: **5radical23dichlorothiophene.out**

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

==========

g3b3
#N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
#N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
#N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
#N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge

Pointgroup= C1 Stoichiometry= C4HCl2S(2) C1[X(C4HCl2S)] #Atoms= 8
Charge = 0 Multiplicity = 2

SCF Energy= -1468.57032663 Predicted Change= -6.608230D-08
MP2 Energy= -1470.757248311 Correl. Energy= -2.18692168

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00042	0.00180	[YES]	0.00042	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.420973	-1.759700	0.000078
C	0.080682	-1.918906	0.000031
C	-0.553828	-0.621775	-0.000049
C	0.329342	0.425326	0.000128
S	1.998414	-0.142347	-0.000197
H	-0.464877	-2.853946	0.000072
Cl	-0.023527	2.110398	0.000219
Cl	-2.280753	-0.440878	-0.000104

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1468.57032663 Predicted Change= -6.608230D-08
MP2 Energy= -1470.757248311 MP2 Cor. Energy= -2.18692168
Zero-point correction (ZPE)= -1471.4518 0.03541
Internal Energy (U)= -1471.4453 0.04191
Enthalpy (H)= -1471.4444 0.04285
Gibbs Free Energy (G)= -1471.4844 0.00278

Frequencies -- 155.1115 173.7482 195.9047

Bromine Radical: B3LYP/6-31g(d)
Supporting Information: bromineradical.out

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt freq ub3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= Br(2)   OH[O(Br)]  #Atoms= 1
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -2571.65691822     Predicted Change=  0.000000D+00
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type       X          Y       Z
---------------------------------------------------------------------
      Br       0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -2571.65691822 Predicted Change=  0.000000D+00
 Zero-point correction (ZPE)=        -2571.6569  0.00000
 Internal Energy (U)=               -2571.6555  0.00141
 Enthalpy (H)=                      -2571.6545   0.00236
 Gibbs Free Energy (G)=             -2571.6737   -0.01683
---------------------------------------------------------------------
```

Chlorine Radical: B3LYP/6-31g(d)
Supporting Information: chlorineradical_ub3lyp631gd.out

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= Cl(2)   OH[O(Cl)]  #Atoms= 1
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -460.136242222     Predicted Change=  0.000000D+00
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type       X           Y       Z
---------------------------------------------------------------------
      Cl        0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -460.136242222 Predicted Change=  0.000000D+00
 Zero-point correction (ZPE)=         -460.1362  0.00000
 Internal Energy (U)=                 -460.1348  0.00141
 Enthalpy (H)=                       -460.1338   0.00236
 Gibbs Free Energy (G)=               -460.1519   -0.01567
---------------------------------------------------------------------
```

Fluorine Radical: B3LYP/6-31g(d)
Supporting Information: fluorineradical.out

```
---------------------------------------------------------------------
 Using  Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt freq nosymm ub3lyp/6-31g(d) geom=connectivity scf=maxcycle=5000
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= F(2)   OH[O(F)]  #Atoms= 1
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -99.7155363805     Predicted Change=  0.000000D+00
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type       X           Y       Z
---------------------------------------------------------------------
      F       -1.233766       1.103896       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -99.7155363805 Predicted Change=  0.000000D+00
 Zero-point correction (ZPE)=          -99.7155  0.00000
 Internal Energy (U)=                  -99.7141  0.00141
 Enthalpy (H)=                        -99.7131   0.00236
 Gibbs Free Energy (G)=                -99.7303   -0.01481
---------------------------------------------------------------------
```

Hydrogen Radical: B3LYP/6-31g(d)
Supporting Information: hydrogenrad.out

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # opt=(modredundant) freq ub3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= H(2)   OH[O(H)]  #Atoms= 1
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -0.500272784191    Predicted Change=  0.000000D+00
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type       X           Y       Z
---------------------------------------------------------------------
      H         0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -0.500272784191       Predicted Change=  0.000000D+00
 Zero-point correction (ZPE)=           -0.5002  0.00000
 Internal Energy (U)=                  -0.4988  0.00141
 Enthalpy (H)=                        -0.4979   0.00236
 Gibbs Free Energy (G)=                -0.5109   -0.01065
---------------------------------------------------------------------
```

Chlorine Radical: G3B3

Supporting Information: chlorineradical.out

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # g3b3
 #N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
 #N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
 #N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= Cl(2)   OH[O(Cl)]  #Atoms= 1
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -459.478996995     Predicted Change=  0.000000D+00
 MP2 Energy= -459.9414838608     Correl. Energy= -0.462486865
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
       Type       X           Y       Z
---------------------------------------------------------------------
      Cl        0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -459.478996995 Predicted Change=  0.000000D+00
 MP2 Energy=     -459.9414838608        MP2 Cor. Energy= -0.462486865
 Zero-point correction (ZPE)=          -460.1362  0.00000
 Internal Energy (U)=                  -460.1348  0.00141
 Enthalpy (H)=                        -460.1338   0.00236
 Gibbs Free Energy (G)=               -460.1519   -0.01567
---------------------------------------------------------------------
```

Hydrogen Radical: B3LYP/6-31g(d)
Supporting Information: hydrogenrad.out

```
---------------------------------------------------------------------
 Using  Gaussian 03:  IA32L-G03RevC.02 12-Jun-2004
=====================================================================
 # g3b3
 #N Geom=AllCheck Guess=Read SCRF=Check B3LYP/6-31G(d) Freq
 #N Geom=AllCheck Guess=Read SCRF=Check QCISD(T,E4T)/6-31G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31+G(d)
 #N Geom=AllCheck Guess=Read SCRF=Check MP4/6-31G(2df,p)
 #N Geom=AllCheck Guess=Read SCRF=Check MP2=Full/GTLarge
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= H(2)   OH[O(H)]  #Atoms= 1
 Charge = 0     Multiplicity = 2
---------------------------------------------------------------------
 SCF Energy= -0.499817915630    Predicted Change=  0.000000D+00
 MP2 Energy= -0.4998179156304    Correl. Energy= 0
=====================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type       X          Y       Z
---------------------------------------------------------------------
      H         0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -0.499817915630       Predicted Change=  0.000000D+00
 MP2 Energy=     -0.4998179156304       MP2 Cor. Energy= 0
 Zero-point correction (ZPE)=           -0.5002  0.00000
 Internal Energy (U)=                  -0.4988  0.00141
 Enthalpy (H)=                        -0.4979   0.00236
 Gibbs Free Energy (G)=                -0.5109   -0.01065
---------------------------------------------------------------------
```